wwPDB X-ray Structure Validation Summary Report (i)

Mar 18, 2024 – 10:09 AM JST

PDB ID	:	8K1R
Title	:	YeeE(TsuA)-YeeD(TsuB) complex for thiosulfate uptake
Authors	:	Ikei, M.; Miyazaki, R.; Monden, K.; Naito, Y.; Takeuchi, A.; Takahashi, Y.S.; Tanaka, Y.; Ichikawa, M.; Tsukazaki, T.
Deposited on	:	2023-07-11
Resolution	:	2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

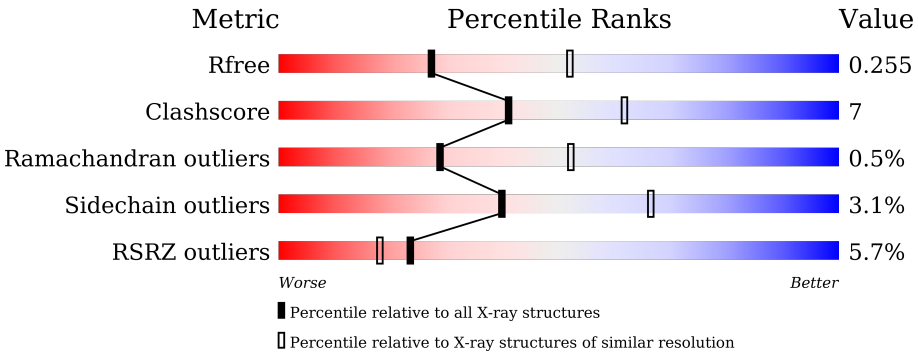
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	460	3% 72% 16% • 11%
1	B	460	7% 74% 13% • 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	OLC	A	503	-	-	-	X
2	OLC	A	511	-	-	-	X
2	OLC	A	512	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6900 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

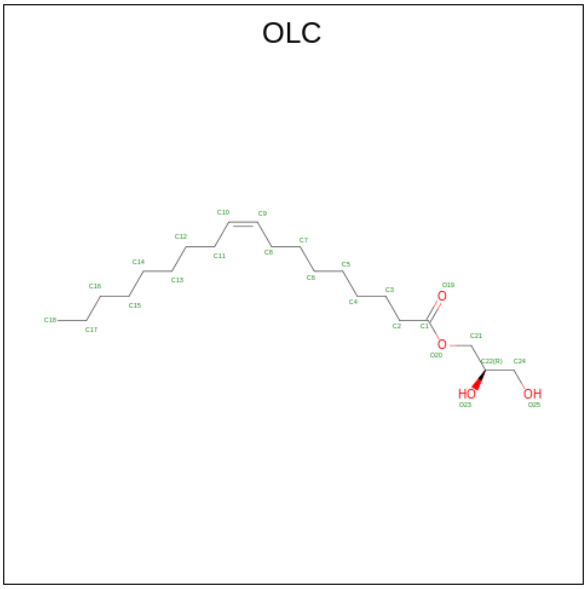
- Molecule 1 is a protein called Spirochaeta thermophila YeeE(TsuA)-YeeD(TsuB),UPF0033 domain-containing protein, SirA-like domain-containing protein (chimera).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	406	Total	C	N	O	S	0	1	0
			3117	2066	504	535	12			
1	A	408	Total	C	N	O	S	0	1	0
			3130	2073	507	538	12			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	22	ALA	CYS	engineered mutation	UNP G0GAP6
B	415	ALA	LEU	engineered mutation	UNP G0GAP7
B	451	GLY	-	expression tag	UNP G0GAP7
B	452	SER	-	expression tag	UNP G0GAP7
B	453	SER	-	expression tag	UNP G0GAP7
B	454	GLY	-	expression tag	UNP G0GAP7
B	455	GLU	-	expression tag	UNP G0GAP7
B	456	ASN	-	expression tag	UNP G0GAP7
B	457	LEU	-	expression tag	UNP G0GAP7
B	458	TYR	-	expression tag	UNP G0GAP7
B	459	PHE	-	expression tag	UNP G0GAP7
B	460	GLN	-	expression tag	UNP G0GAP7
A	22	ALA	CYS	engineered mutation	UNP G0GAP6
A	415	ALA	LEU	engineered mutation	UNP G0GAP7
A	451	GLY	-	expression tag	UNP G0GAP7
A	452	SER	-	expression tag	UNP G0GAP7
A	453	SER	-	expression tag	UNP G0GAP7
A	454	GLY	-	expression tag	UNP G0GAP7
A	455	GLU	-	expression tag	UNP G0GAP7
A	456	ASN	-	expression tag	UNP G0GAP7
A	457	LEU	-	expression tag	UNP G0GAP7
A	458	TYR	-	expression tag	UNP G0GAP7
A	459	PHE	-	expression tag	UNP G0GAP7
A	460	GLN	-	expression tag	UNP G0GAP7

- Molecule 2 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 21 19 2	0	0
2	B	1	Total C O 25 21 4	0	0
2	B	1	Total C 14 14	0	0
2	B	1	Total C 16 16	0	0
2	B	1	Total C O 25 21 4	0	0
2	B	1	Total C O 25 21 4	0	0
2	B	1	Total C O 25 21 4	0	0
2	B	1	Total C O 25 21 4	0	0
2	B	1	Total C O 25 21 4	0	0
2	B	1	Total C O 16 12 4	0	0
2	B	1	Total C 14 14	0	0
2	B	1	Total C 7 7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 21 19 2	0	0
2	A	1	Total C O 22 18 4	0	0
2	A	1	Total C O 25 21 4	0	0
2	A	1	Total C 12 12	0	0
2	A	1	Total C O 25 21 4	0	0
2	A	1	Total C O 25 21 4	0	0
2	A	1	Total C O 25 21 4	0	0
2	A	1	Total C O 25 21 4	0	0
2	A	1	Total C O 25 21 4	0	0
2	A	1	Total C 17 17	0	0
2	A	1	Total C O 25 21 4	0	0
2	A	1	Total C O 25 21 4	0	0
2	A	1	Total C O 20 18 2	0	0
2	A	1	Total C O 15 11 4	0	0

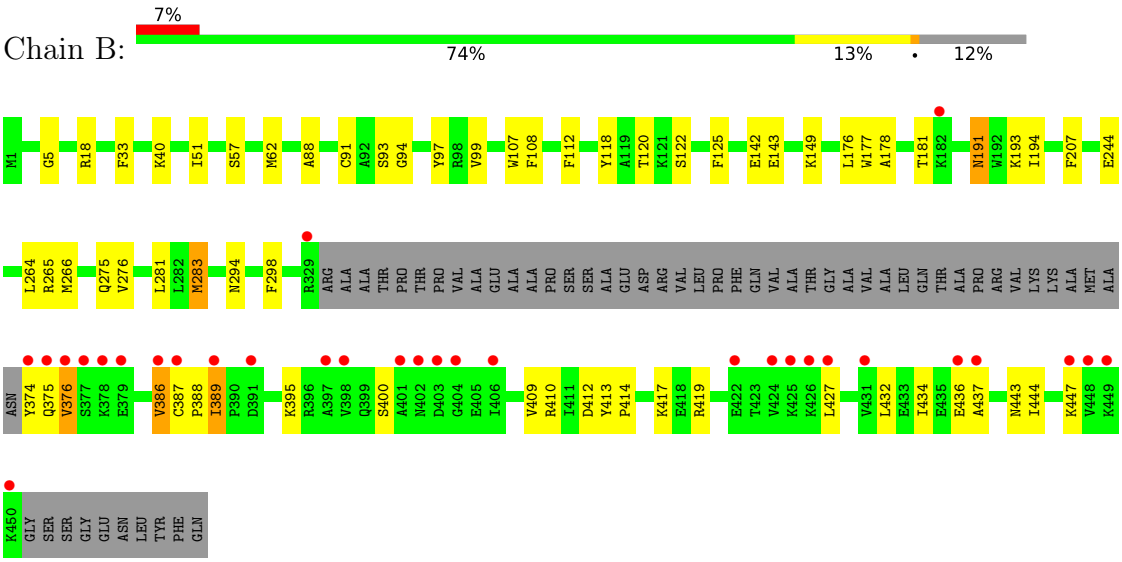
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	51	Total O 51 51	0	0
3	A	57	Total O 57 57	0	0

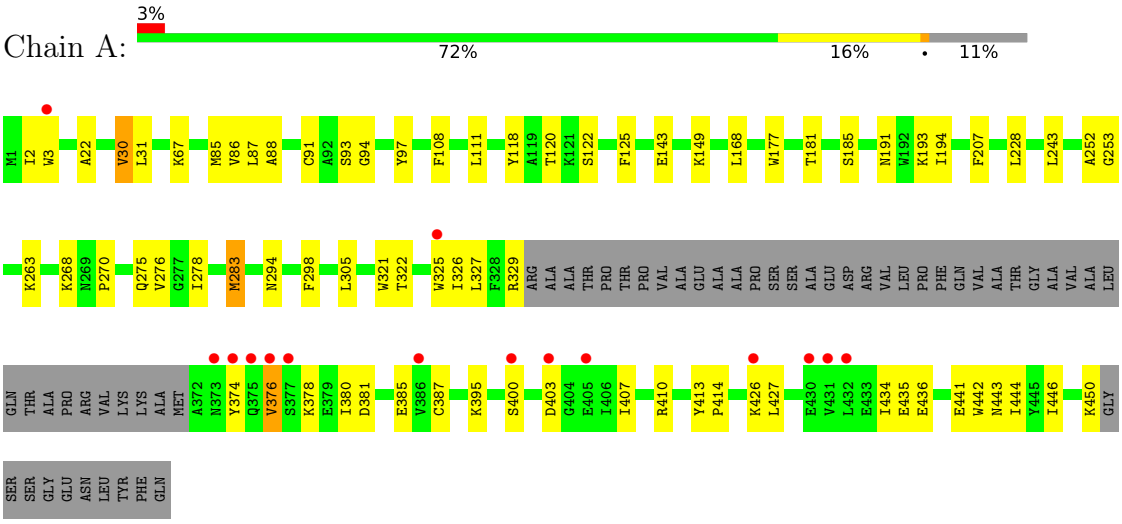
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Spirochaeta thermophila YeeE(TsuA)-YeeD(TsuB),UPF0033 domain-containing protein, SirA-like domain-containing protein (chimera)



• Molecule 1: Spirochaeta thermophila YeeE(TsuA)-YeeD(TsuB),UPF0033 domain-containing protein, SirA-like domain-containing protein (chimera)



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α, β, γ	73.58Å 101.75Å 182.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.93 – 2.60 49.93 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.93-2.60) 71.7 (49.93-2.31)	Depositor EDS
R_{merge}	0.99	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	-0.17 (at 2.32Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.206 , 0.253 0.208 , 0.255	Depositor DCC
R_{free} test set	19868 reflections (32.66%)	wwPDB-VP
Wilson B-factor (Å^2)	21.5	Xtriage
Anisotropy	0.792	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 56.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6900	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.72 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.2129e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OLC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.43	0/3210	0.56	1/4363 (0.0%)
1	B	0.42	0/3197	0.57	1/4345 (0.0%)
All	All	0.43	0/6407	0.56	2/8708 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	283	MET	CG-SD-CE	-7.73	87.83	100.20
1	A	283	MET	CG-SD-CE	-7.12	88.80	100.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	387	CYS	Peptide
1	B	386	VAL	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3130	0	3214	53	0
1	B	3117	0	3203	35	0
2	A	307	0	488	20	0
2	B	238	0	386	8	0
3	A	57	0	0	3	0
3	B	51	0	0	1	0
All	All	6900	0	7291	100	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 100 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:CYS:HA	1:B:283:MET:HE1	1.50	0.91
1:A:325:TRP:HB2	2:A:510:OLC:H7A	1.65	0.78
1:A:91:CYS:HA	1:A:283:MET:HE3	1.68	0.76
1:B:143:GLU:HB2	1:B:149:LYS:HB2	1.71	0.72
1:B:266:MET:HG3	1:A:270:PRO:HG3	1.71	0.72

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	405/460 (88%)	390 (96%)	14 (4%)	1 (0%)	47 71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	403/460 (88%)	392 (97%)	8 (2%)	3 (1%)	22 43
All	All	808/920 (88%)	782 (97%)	22 (3%)	4 (0%)	29 52

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	375	GLN
1	B	437	ALA
1	A	376	VAL
1	B	376	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	321/358 (90%)	312 (97%)	9 (3%)	43 69
1	B	320/358 (89%)	309 (97%)	11 (3%)	37 63
All	All	641/716 (90%)	621 (97%)	20 (3%)	40 66

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	SER
1	A	305	LEU
1	A	400	SER
1	A	378	LYS
1	B	207	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	24	ASN
1	B	294	ASN
1	A	191	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

26 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	OLC	A	503	-	24,24,24	0.22	0	25,25,25	0.26	0
2	OLC	A	501	-	20,20,24	0.26	0	20,20,25	0.24	0
2	OLC	A	508	-	24,24,24	0.28	0	25,25,25	0.27	0
2	OLC	A	514	-	14,14,24	0.23	0	15,15,25	0.40	0
2	OLC	A	505	-	24,24,24	0.25	0	25,25,25	0.26	0
2	OLC	A	512	-	24,24,24	0.22	0	25,25,25	0.38	0
2	OLC	B	509	-	24,24,24	0.22	0	25,25,25	0.27	0
2	OLC	A	507	-	24,24,24	0.26	0	25,25,25	0.36	0
2	OLC	A	513	-	19,19,24	0.31	0	19,19,25	0.44	0
2	OLC	A	509	-	24,24,24	0.25	0	25,25,25	0.30	0
2	OLC	B	511	-	13,13,24	0.21	0	12,12,25	0.31	0
2	OLC	B	502	-	24,24,24	0.29	0	25,25,25	0.35	0
2	OLC	B	506	-	24,24,24	0.24	0	25,25,25	0.29	0
2	OLC	A	511	-	24,24,24	0.24	0	25,25,25	0.34	0
2	OLC	B	503	-	13,13,24	0.20	0	12,12,25	0.23	0
2	OLC	A	502	-	21,21,24	0.34	0	22,22,25	0.31	0
2	OLC	B	504	-	15,15,24	0.21	0	14,14,25	0.20	0
2	OLC	A	504	-	11,11,24	0.15	0	9,10,25	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	OLC	B	510	-	15,15,24	0.22	0	16,16,25	0.28	0
2	OLC	B	505	-	24,24,24	0.27	0	25,25,25	0.26	0
2	OLC	B	512	-	6,6,24	0.16	0	5,5,25	0.13	0
2	OLC	B	507	-	24,24,24	0.22	0	25,25,25	0.32	0
2	OLC	B	501	-	20,20,24	0.35	0	20,20,25	0.22	0
2	OLC	A	506	-	24,24,24	0.26	0	25,25,25	0.25	0
2	OLC	B	508	-	24,24,24	0.26	0	25,25,25	0.26	0
2	OLC	A	510	-	16,16,24	0.19	0	15,15,25	0.27	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	A	503	-	-	0/24/24/24	-
2	OLC	A	501	-	-	4/19/19/24	-
2	OLC	A	508	-	-	3/24/24/24	-
2	OLC	A	514	-	-	6/14/14/24	-
2	OLC	A	505	-	-	7/24/24/24	-
2	OLC	A	512	-	-	6/24/24/24	-
2	OLC	B	509	-	-	4/24/24/24	-
2	OLC	A	507	-	-	5/24/24/24	-
2	OLC	A	513	-	-	7/17/17/24	-
2	OLC	A	509	-	-	4/24/24/24	-
2	OLC	B	511	-	-	5/11/11/24	-
2	OLC	B	502	-	-	5/24/24/24	-
2	OLC	B	506	-	-	4/24/24/24	-
2	OLC	A	511	-	-	10/24/24/24	-
2	OLC	B	503	-	-	0/11/11/24	-
2	OLC	A	502	-	-	7/21/21/24	-
2	OLC	B	504	-	-	2/13/13/24	-
2	OLC	A	504	-	-	1/9/9/24	-
2	OLC	B	510	-	-	1/15/15/24	-
2	OLC	B	505	-	-	5/24/24/24	-
2	OLC	B	512	-	-	0/4/4/24	-
2	OLC	B	507	-	-	1/24/24/24	-
2	OLC	B	501	-	-	4/19/19/24	-
2	OLC	A	506	-	-	6/24/24/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	B	508	-	-	6/24/24/24	-
2	OLC	A	510	-	-	2/14/14/24	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 105 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	505	OLC	C2-C1-O20-C21
2	B	505	OLC	O19-C1-O20-C21
2	B	508	OLC	C2-C1-O20-C21
2	B	508	OLC	O19-C1-O20-C21
2	A	505	OLC	O20-C21-C22-C24

There are no ring outliers.

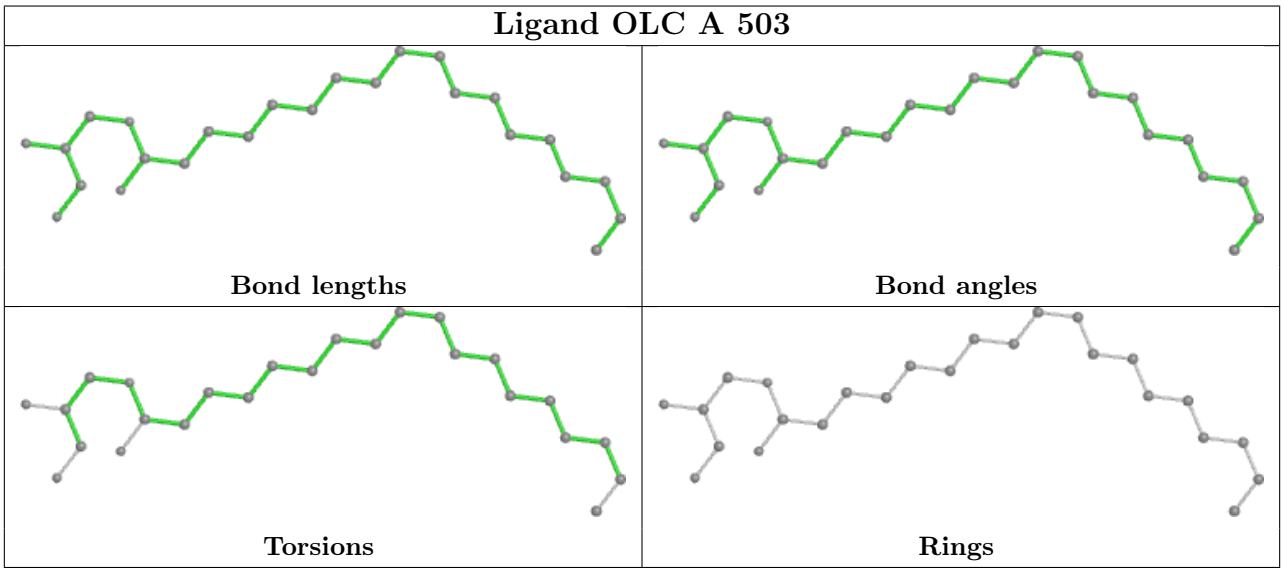
18 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	503	OLC	1	0
2	A	508	OLC	4	0
2	A	505	OLC	4	0
2	A	512	OLC	2	0
2	B	509	OLC	2	0
2	A	507	OLC	1	0
2	A	513	OLC	1	0
2	A	509	OLC	4	0
2	A	511	OLC	3	0
2	B	503	OLC	1	0
2	A	502	OLC	1	0
2	A	504	OLC	1	0
2	B	510	OLC	1	0
2	B	512	OLC	1	0
2	B	507	OLC	2	0
2	B	501	OLC	1	0
2	B	508	OLC	2	0
2	A	510	OLC	3	0

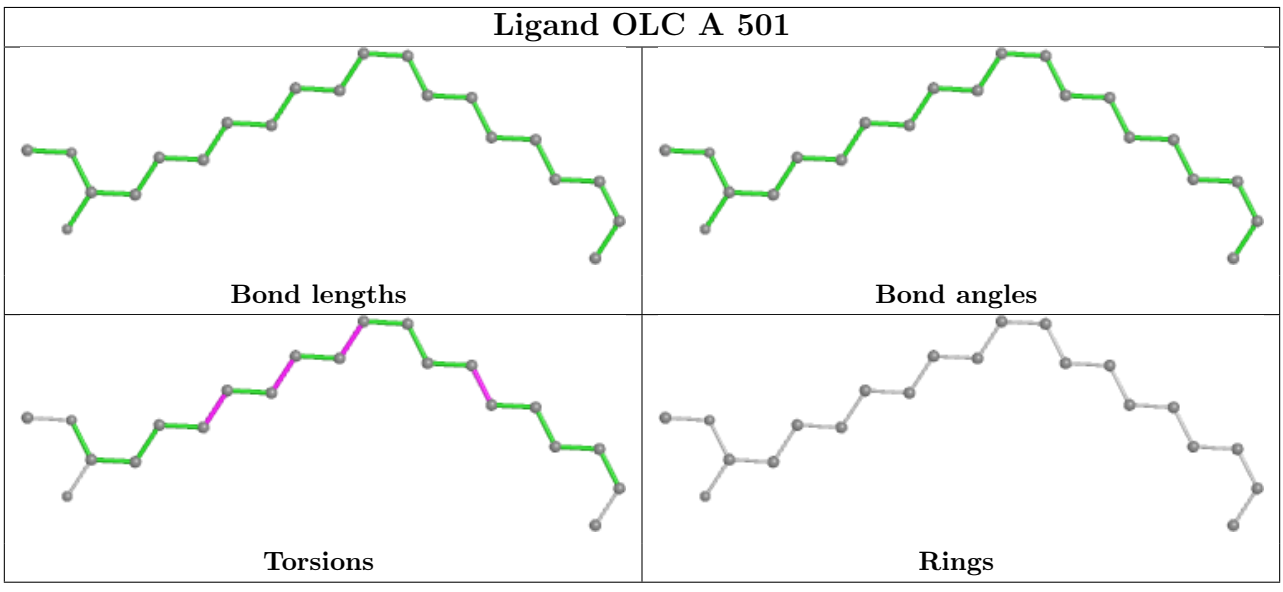
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

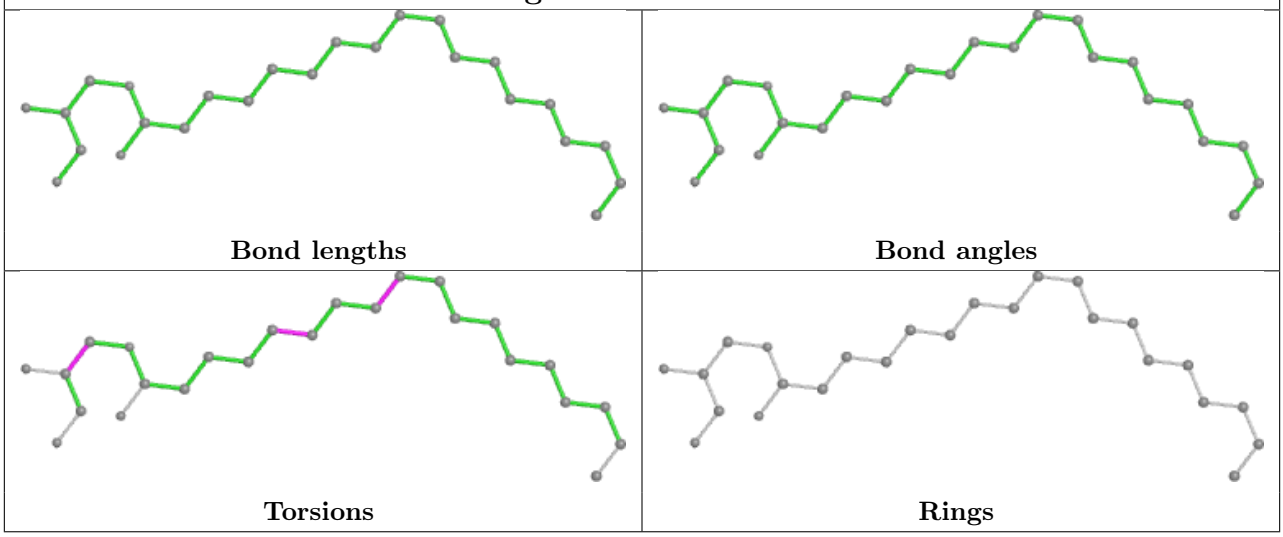
Ligand OLC A 503



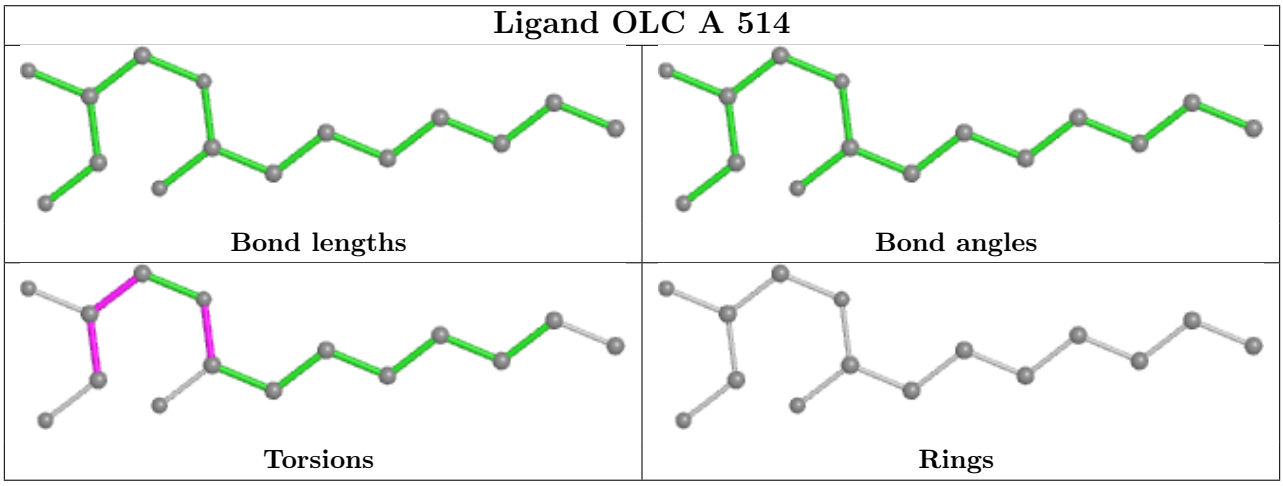
Ligand OLC A 501



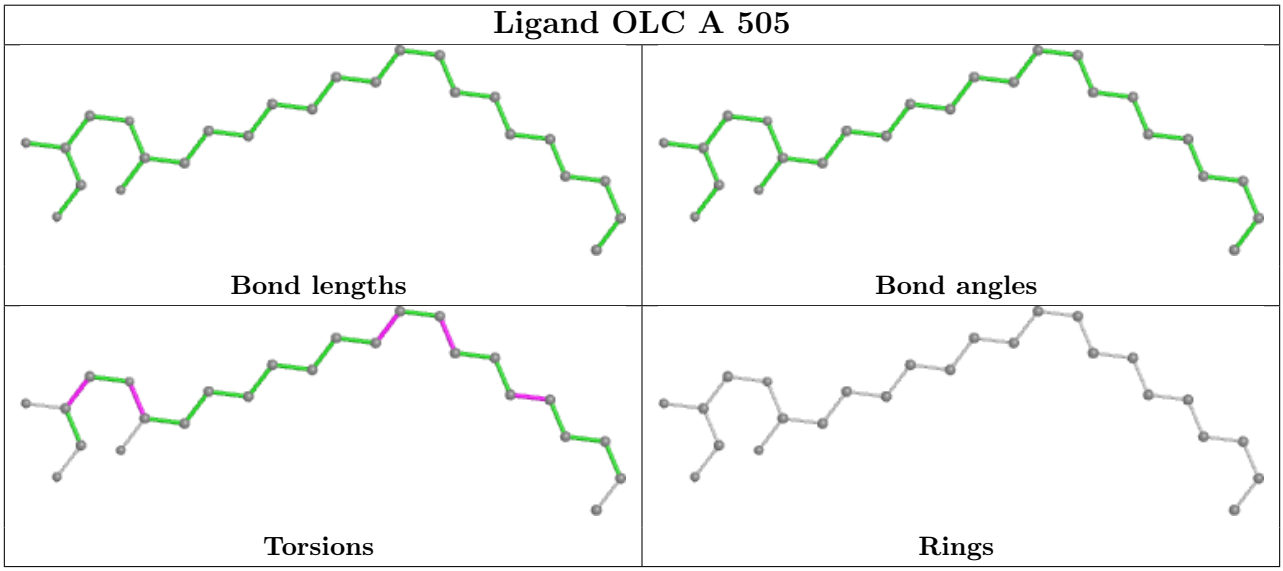
Ligand OLC A 508



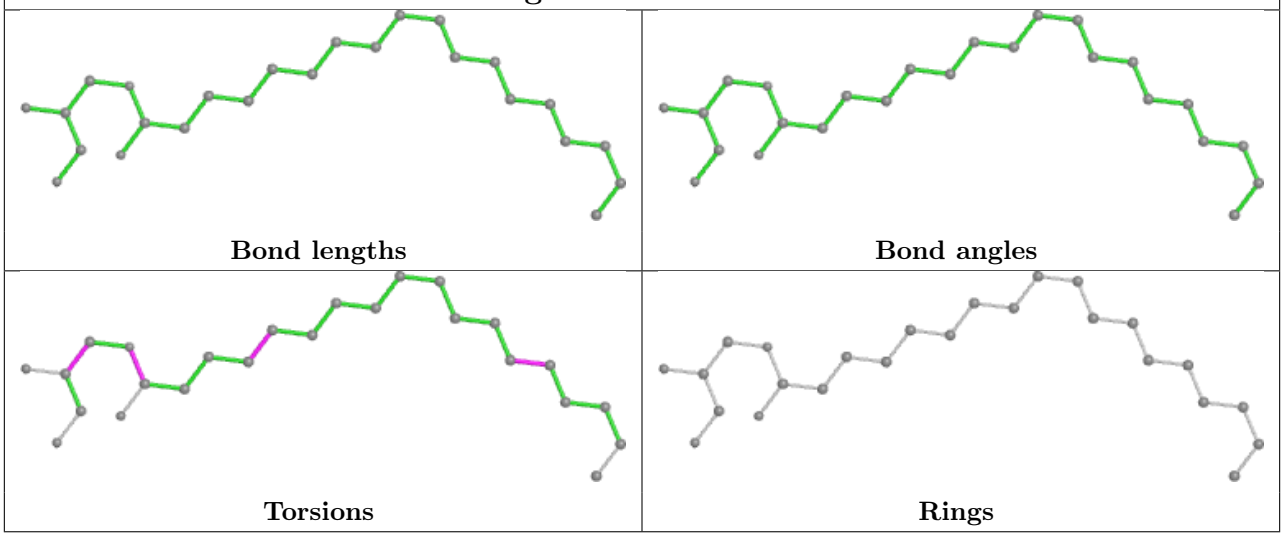
Ligand OLC A 514



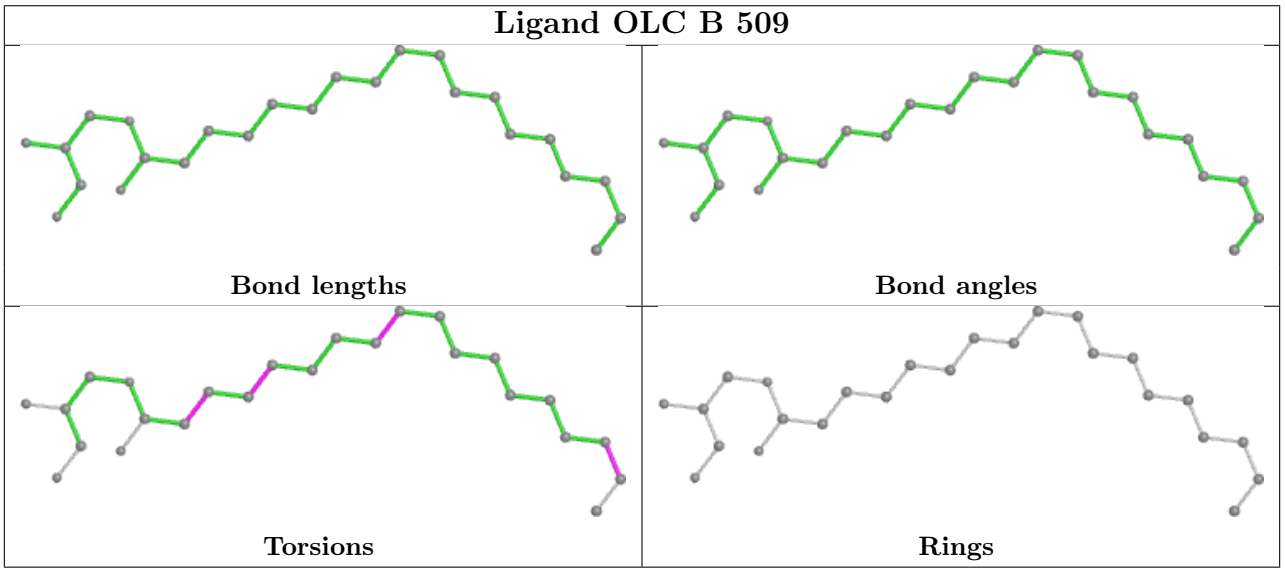
Ligand OLC A 505



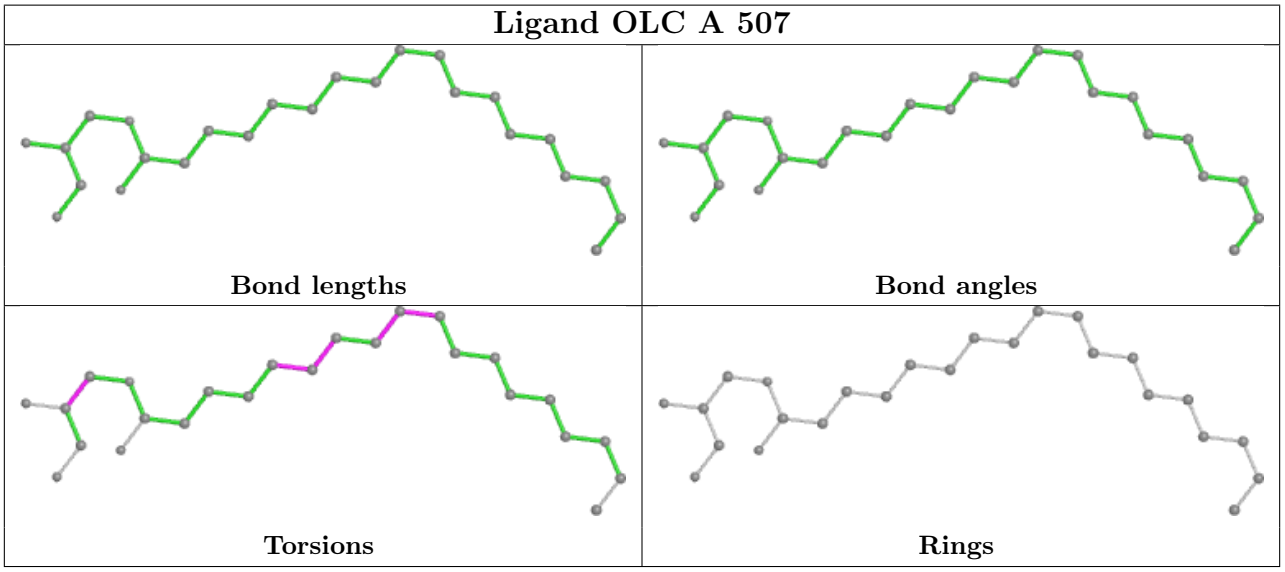
Ligand OLC A 512



Ligand OLC B 509



Ligand OLC A 507



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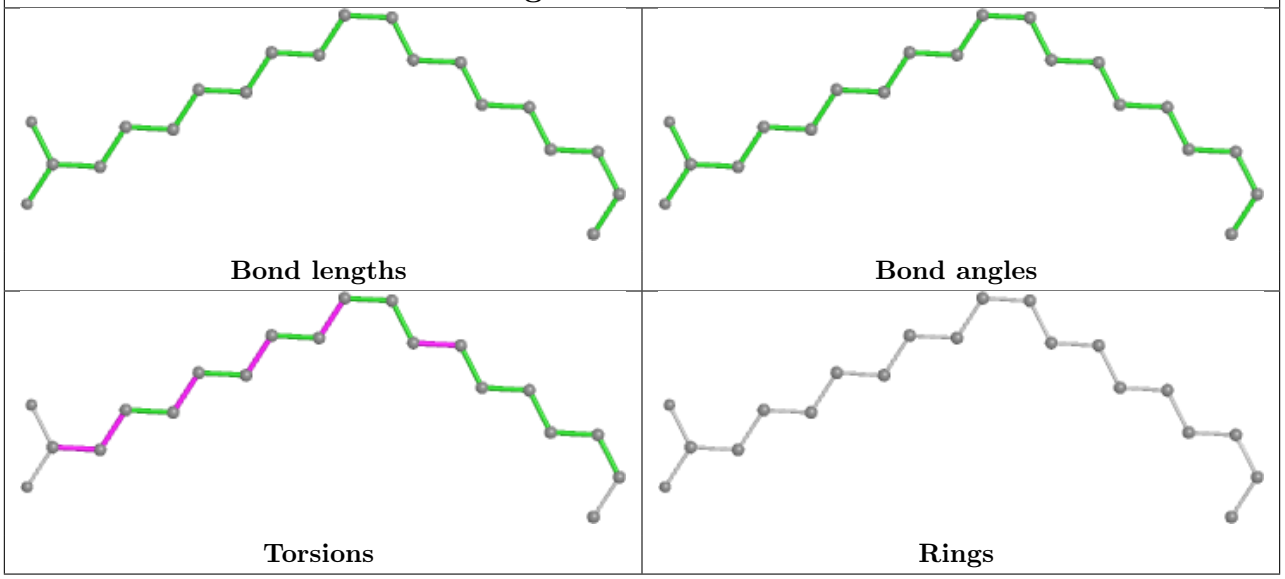

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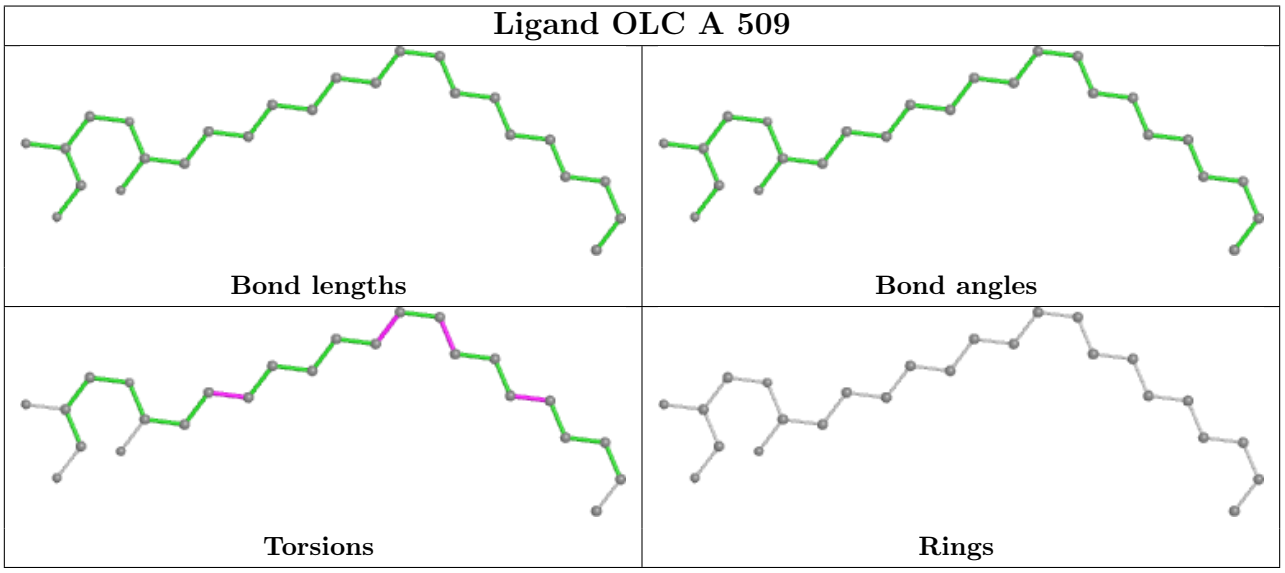
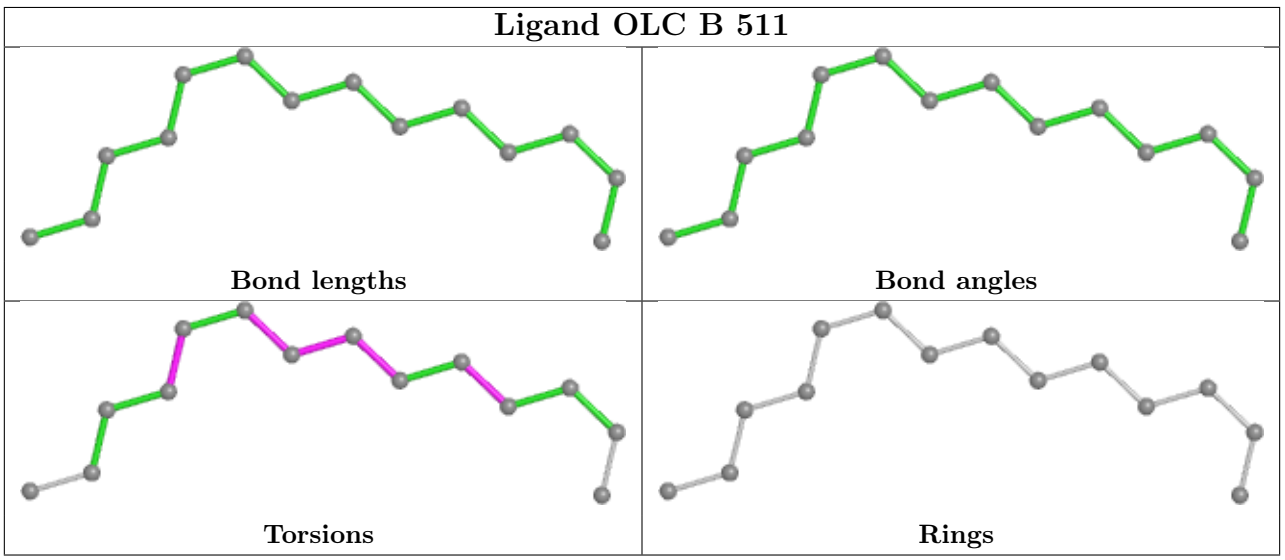
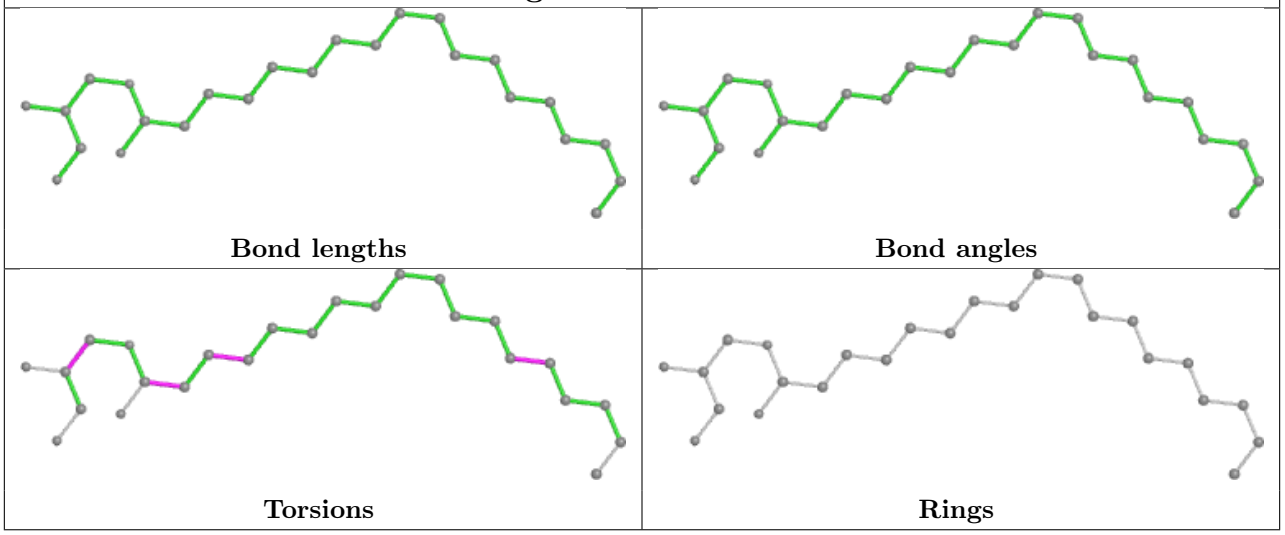


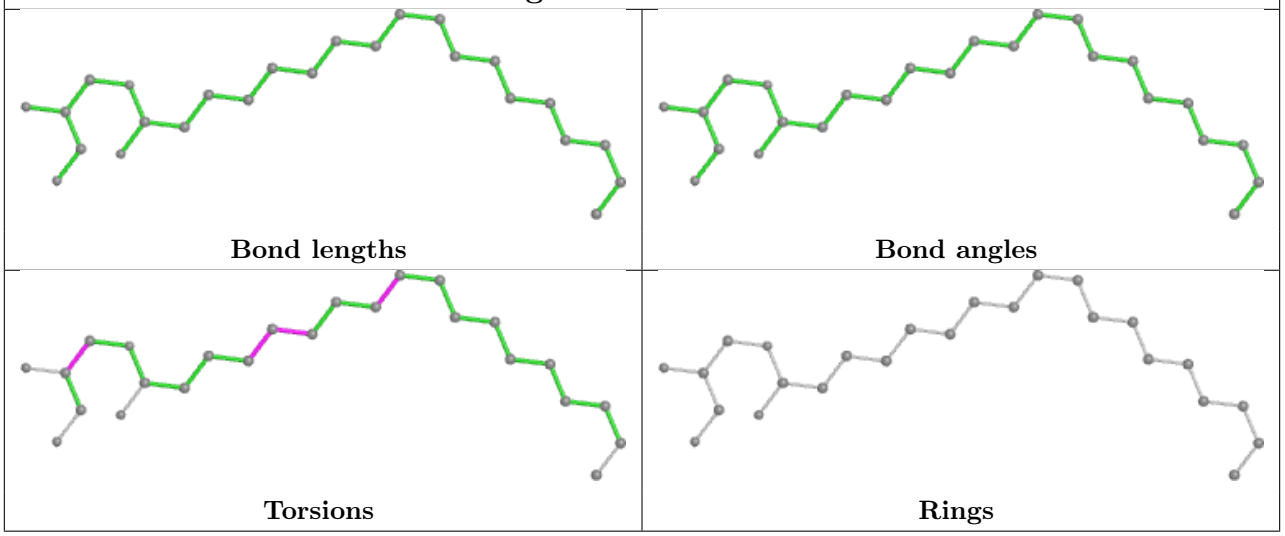
Ligand OLC B 511



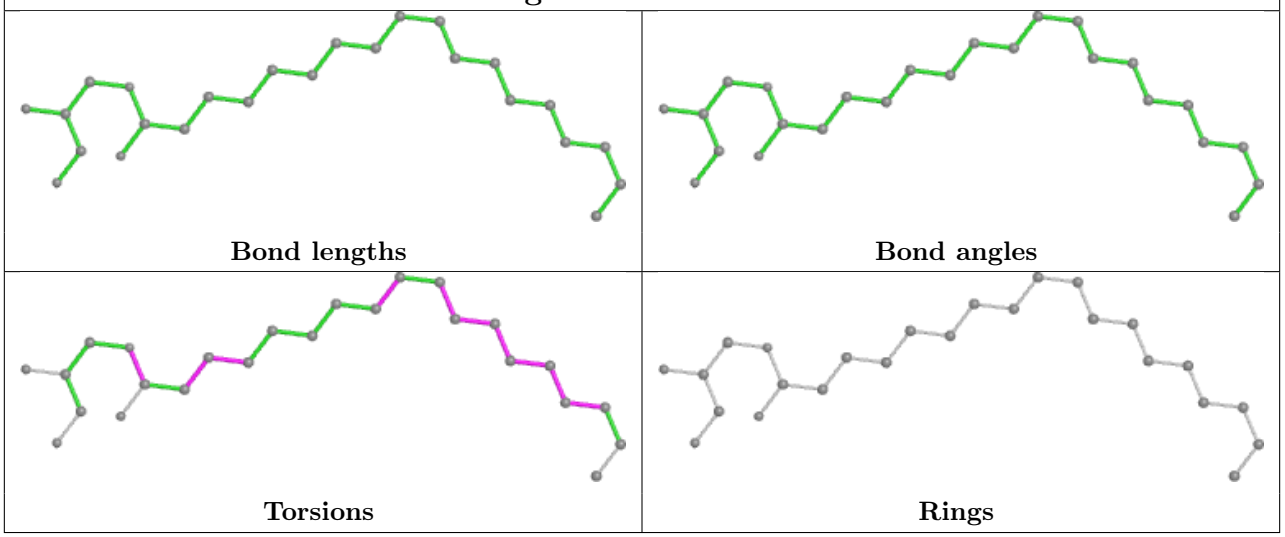
Ligand OLC B 502



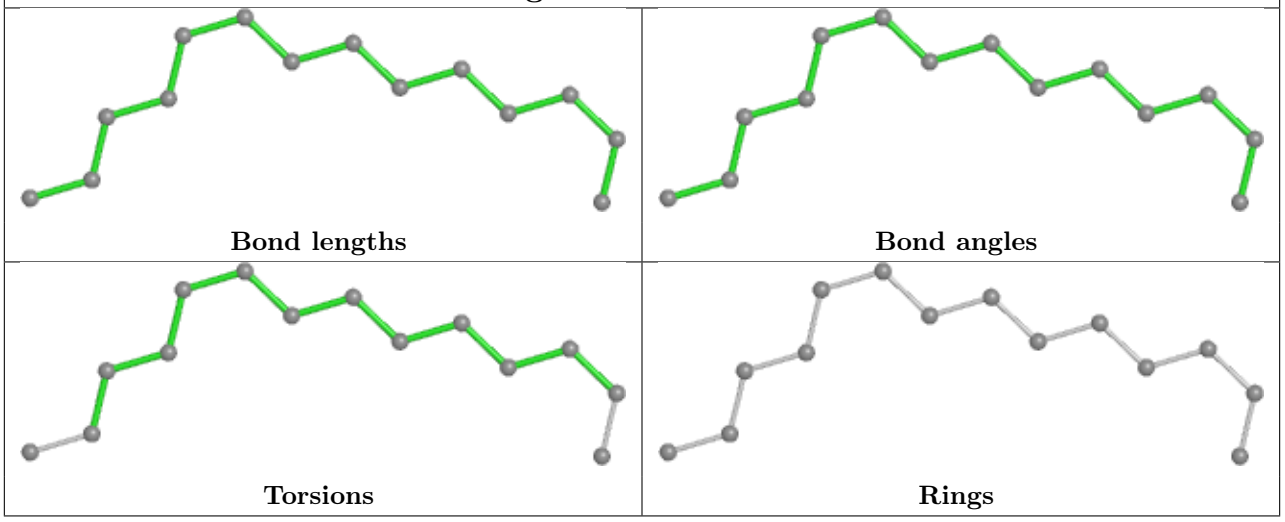
Ligand OLC B 506



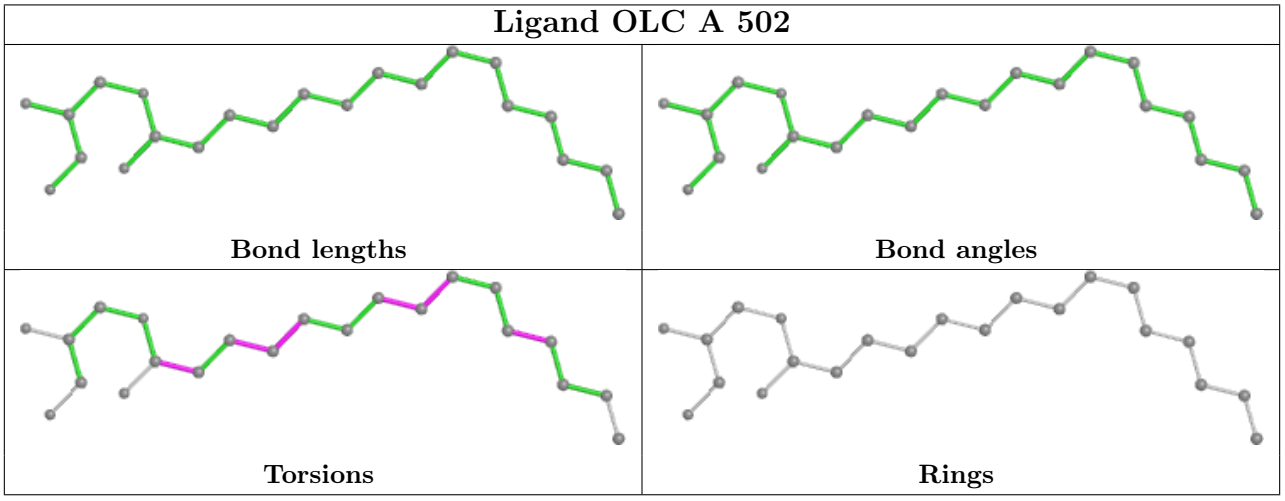
Ligand OLC A 511



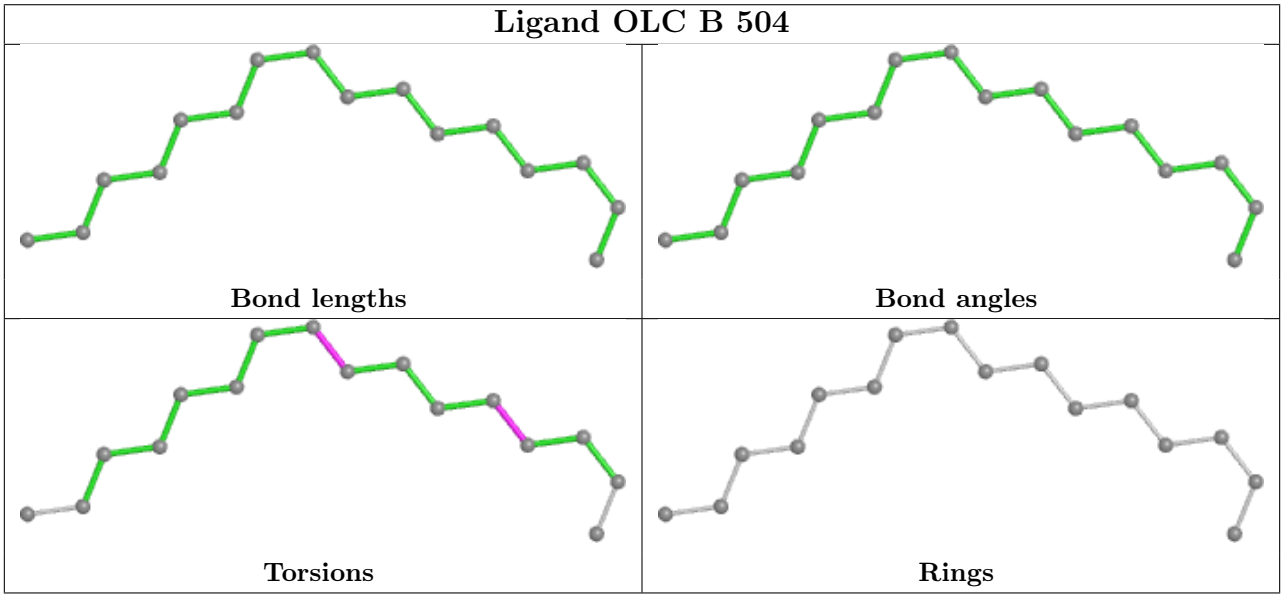
Ligand OLC B 503



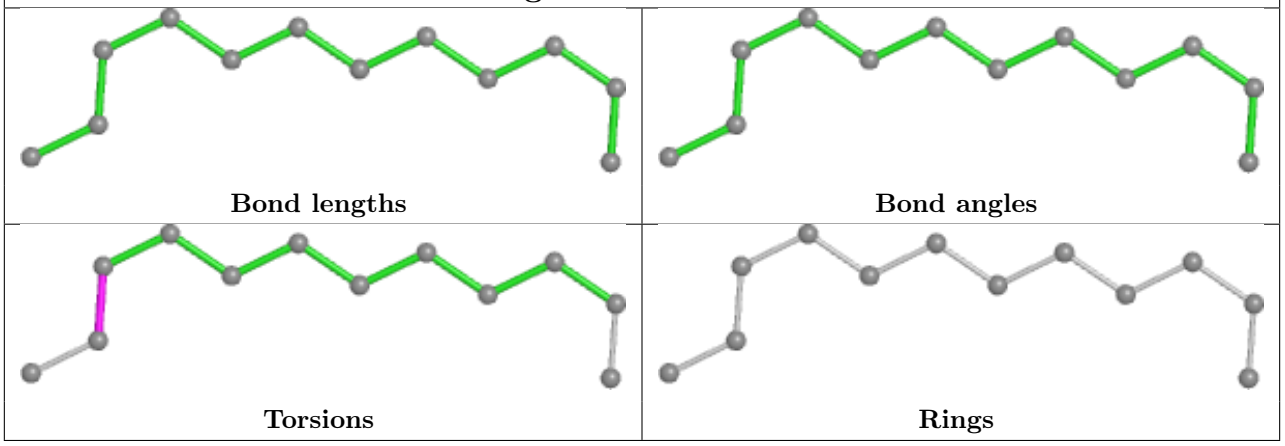
Ligand OLC A 502



Ligand OLC B 504



Ligand OLC A 504



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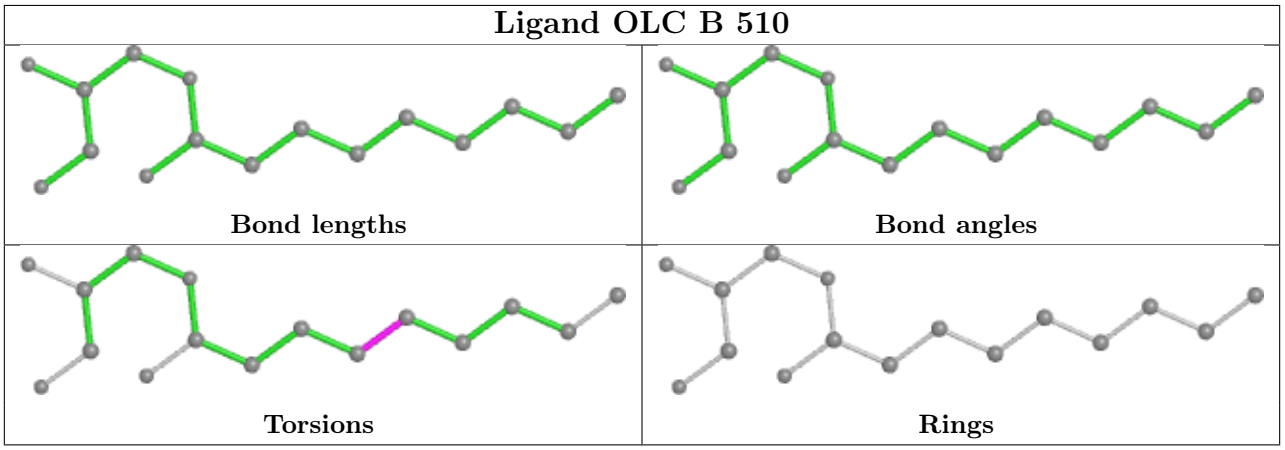

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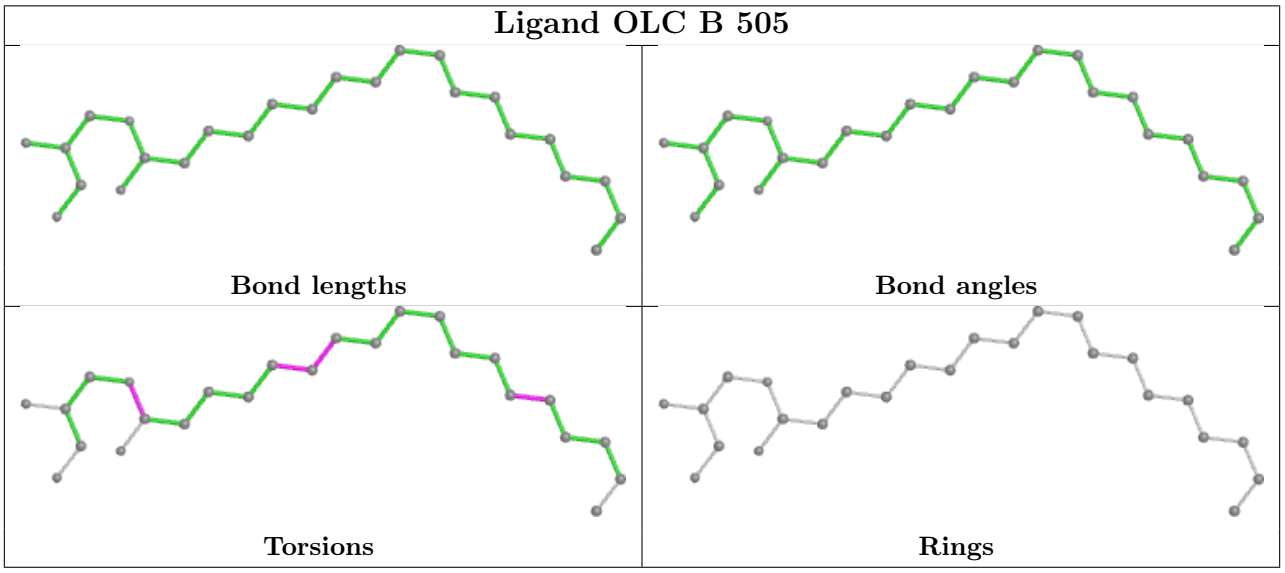

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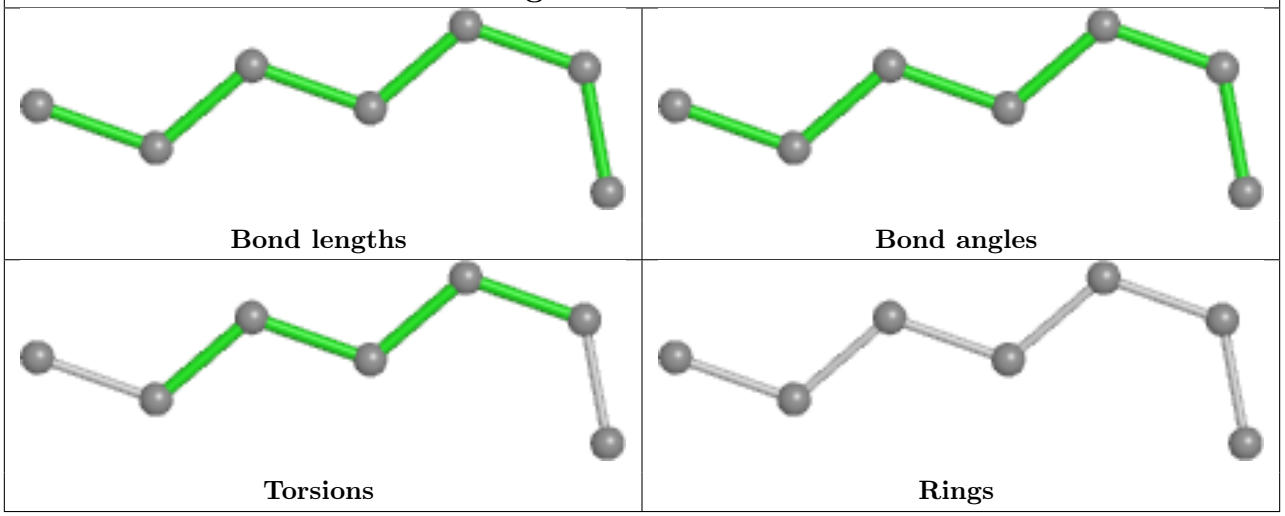

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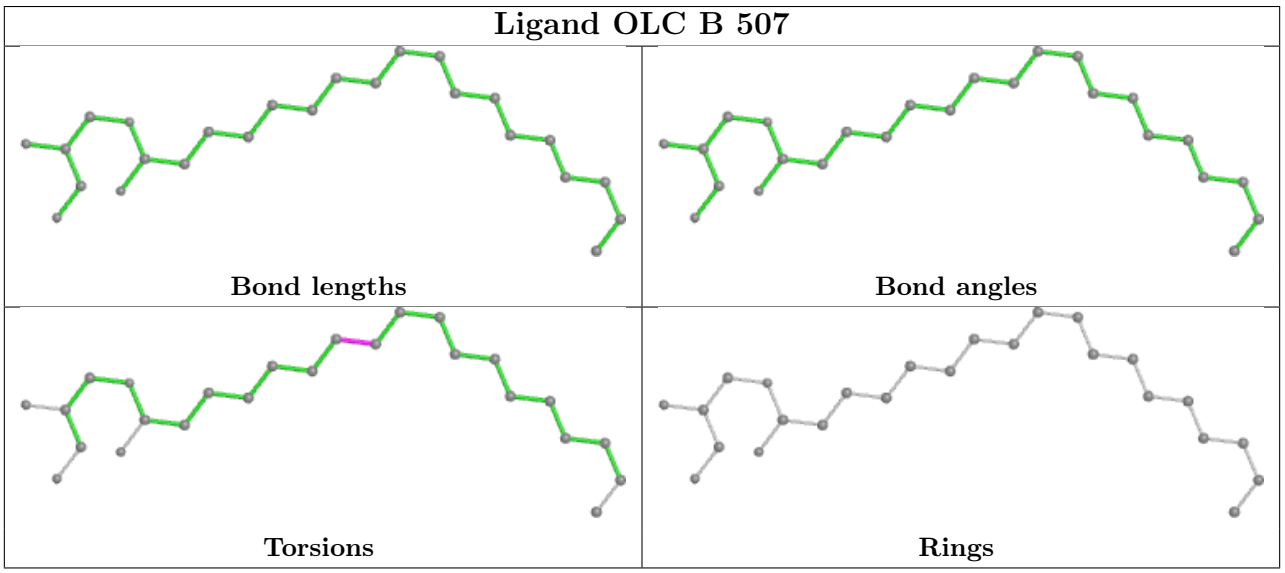

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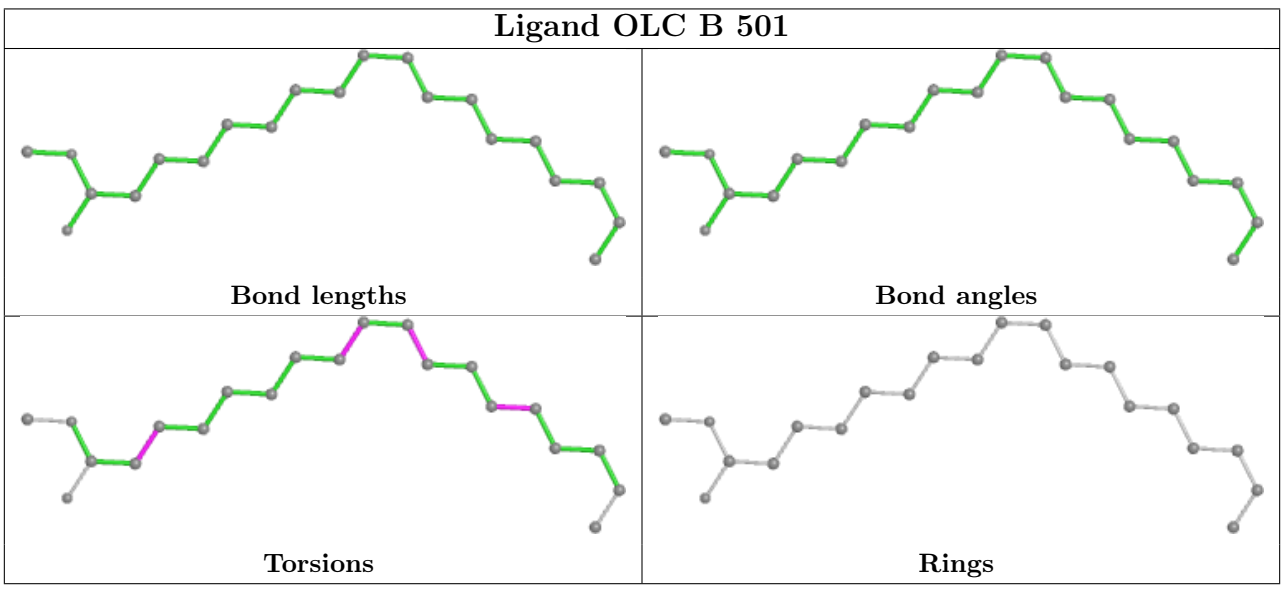

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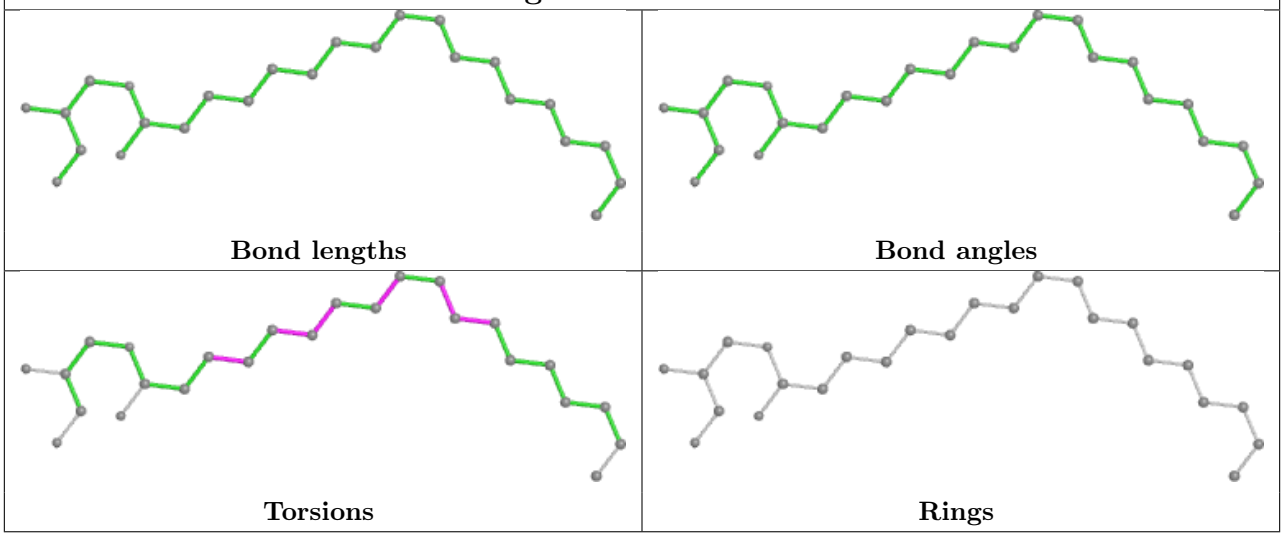

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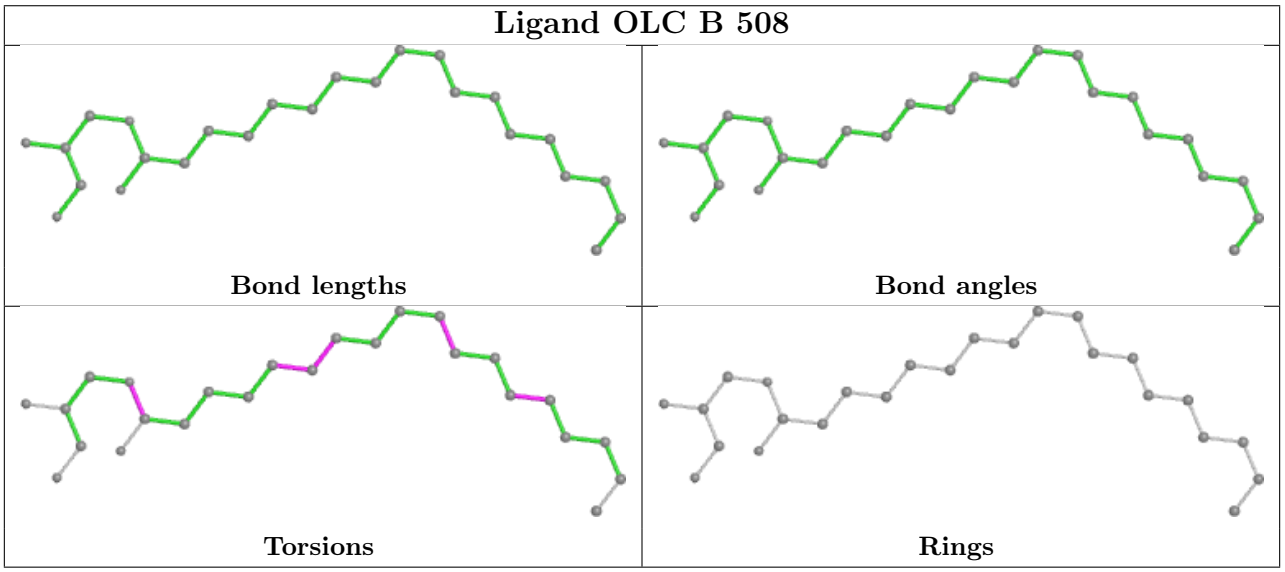

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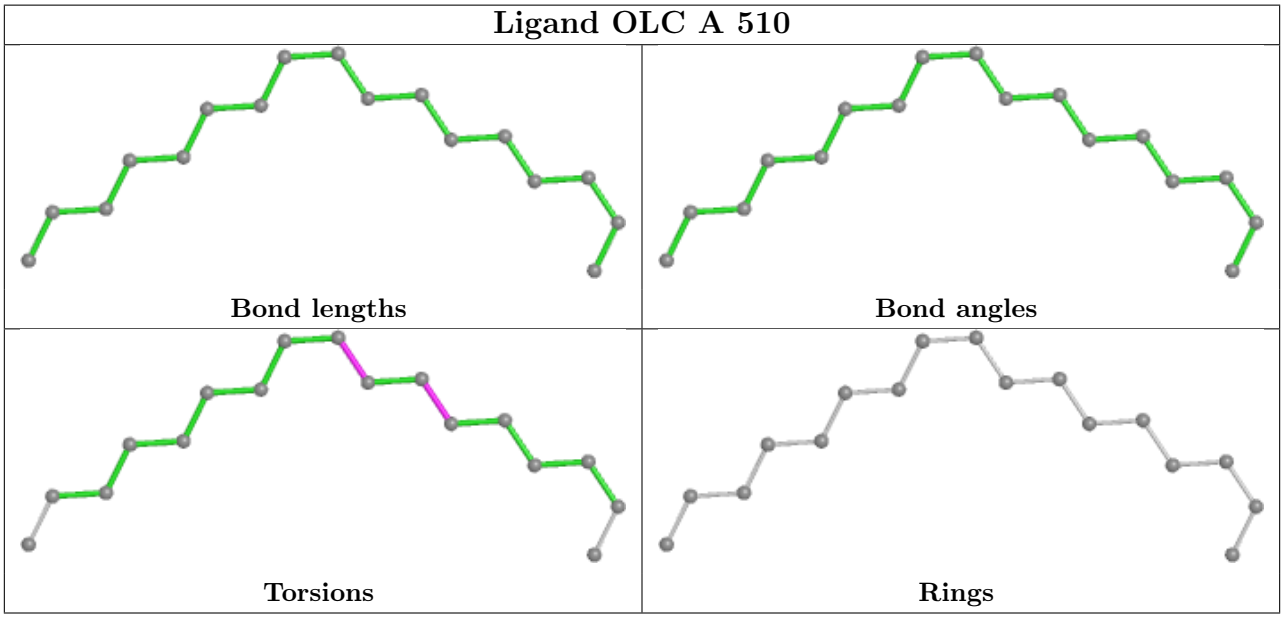


5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	408/460 (88%)	-0.27	15 (3%)	41	34	19, 29, 72, 96	0
1	B	406/460 (88%)	-0.10	31 (7%)	13	10	19, 29, 92, 109	0
All	All	814/920 (88%)	-0.19	46 (5%)	23	18	19, 29, 83, 109	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	386	VAL	11.2
1	A	386	VAL	5.2
1	B	376	VAL	5.2
1	B	406	ILE	4.8
1	B	375	GLN	3.8

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

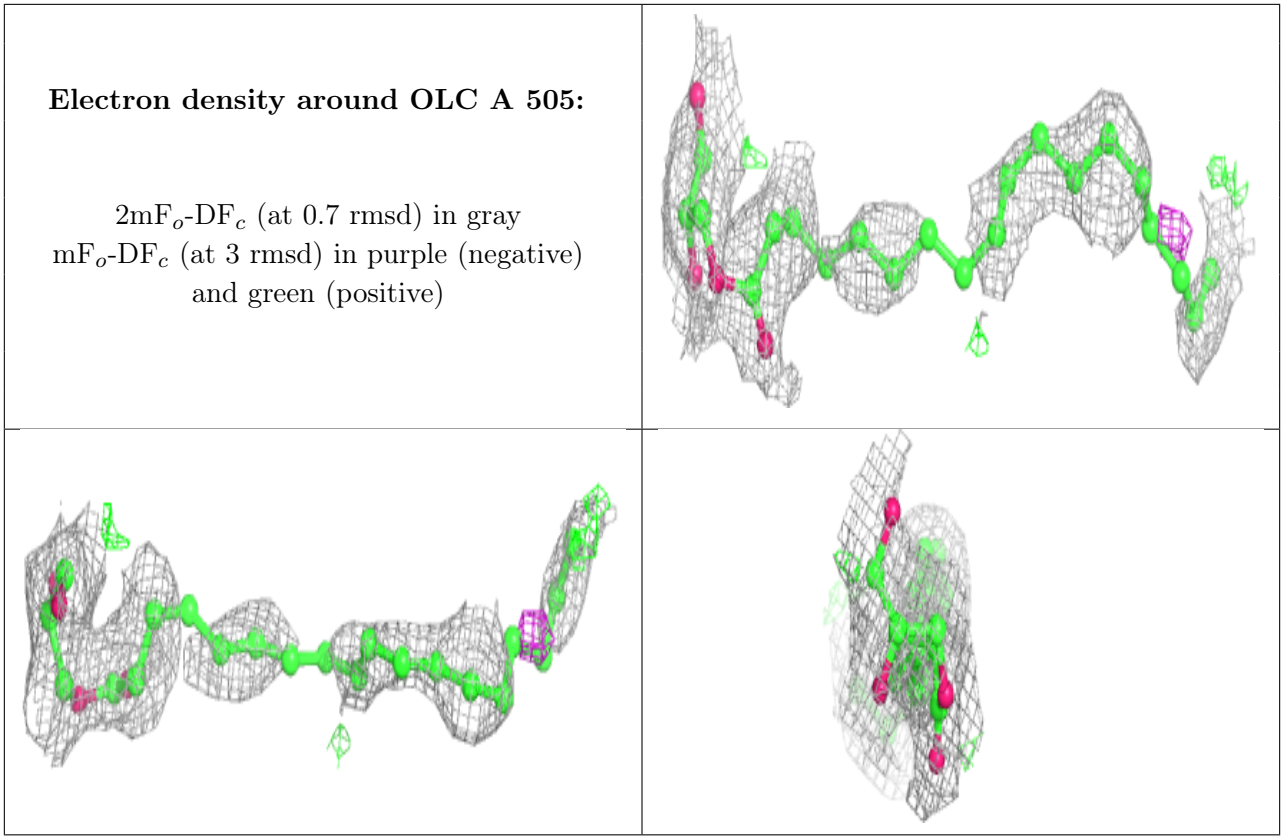
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	OLC	A	505	25/25	0.59	0.34	55,73,82,83	0
2	OLC	A	512	25/25	0.59	0.41	37,58,67,71	0
2	OLC	A	503	25/25	0.61	0.53	53,63,83,89	0
2	OLC	A	504	12/25	0.62	0.26	39,57,75,81	0
2	OLC	A	511	25/25	0.63	0.41	42,57,77,84	0
2	OLC	A	510	17/25	0.65	0.26	26,48,55,57	0
2	OLC	B	511	14/25	0.65	0.32	53,60,75,75	0
2	OLC	B	506	25/25	0.65	0.34	39,58,89,98	0
2	OLC	A	506	25/25	0.66	0.29	31,45,68,84	0
2	OLC	B	505	25/25	0.66	0.32	34,48,68,73	0
2	OLC	B	507	25/25	0.68	0.28	29,43,64,79	0
2	OLC	B	503	14/25	0.68	0.26	45,64,73,78	0
2	OLC	B	504	16/25	0.68	0.27	32,47,52,54	0
2	OLC	A	509	25/25	0.77	0.25	32,43,67,76	0
2	OLC	A	508	25/25	0.78	0.26	36,46,58,61	0
2	OLC	B	512	7/25	0.79	0.24	45,48,51,56	0
2	OLC	A	513	20/25	0.79	0.22	36,52,68,68	0
2	OLC	B	508	25/25	0.81	0.21	32,42,75,77	0
2	OLC	A	507	25/25	0.81	0.21	31,39,49,52	0
2	OLC	A	514	15/25	0.81	0.22	45,55,68,74	0
2	OLC	B	510	16/25	0.83	0.22	47,62,72,75	0
2	OLC	B	501	21/25	0.84	0.23	23,30,44,61	0
2	OLC	A	501	21/25	0.85	0.24	23,31,40,51	0
2	OLC	B	509	25/25	0.86	0.18	29,38,46,53	0
2	OLC	B	502	25/25	0.87	0.19	19,36,52,61	0
2	OLC	A	502	22/25	0.87	0.20	23,28,53,55	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

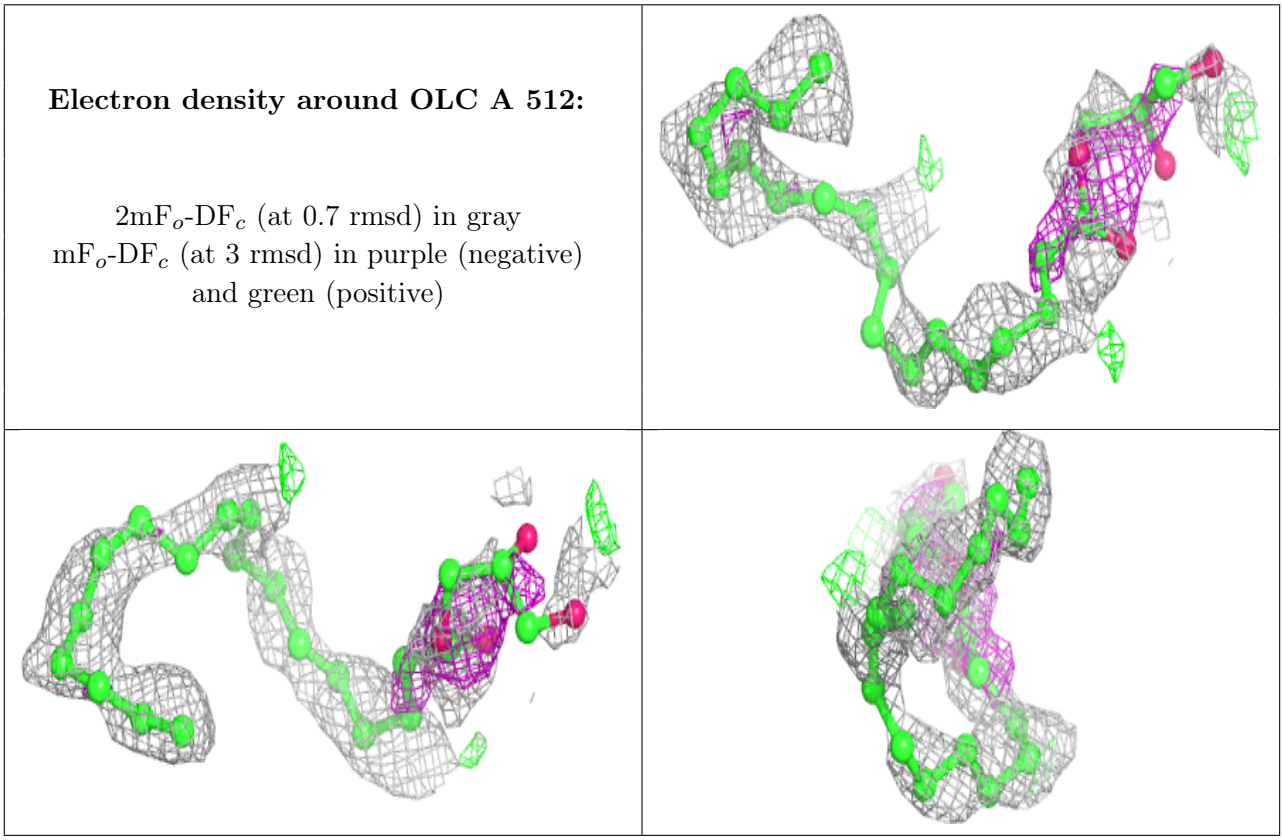
Electron density around OLC A 505:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



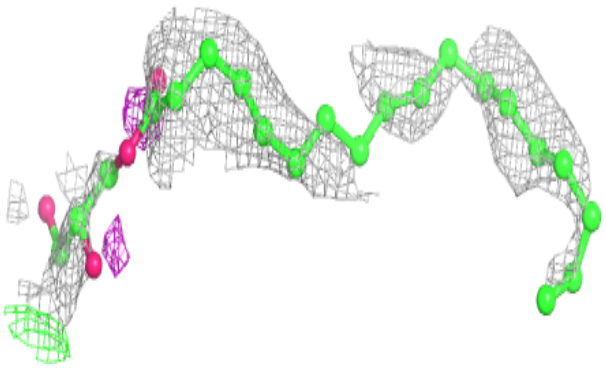
Electron density around OLC A 512:

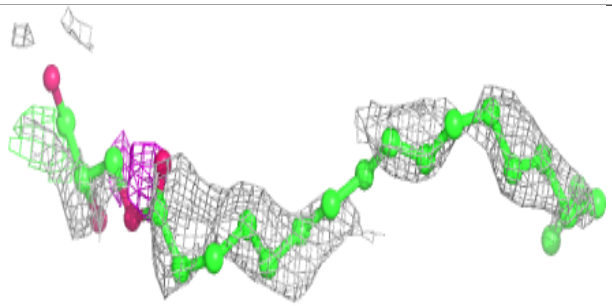
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

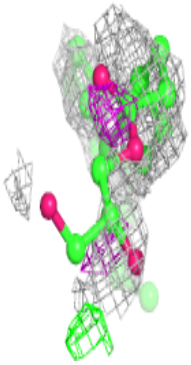


Electron density around OLC A 503:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

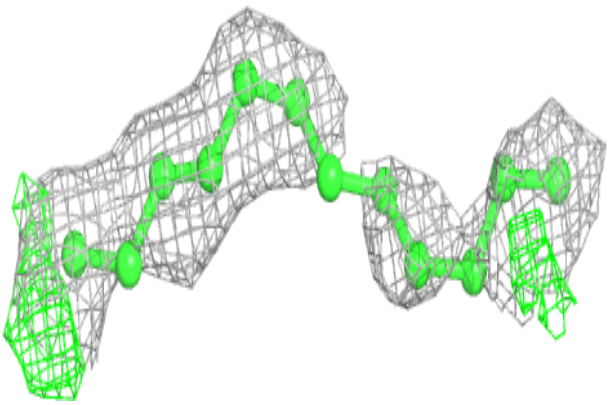


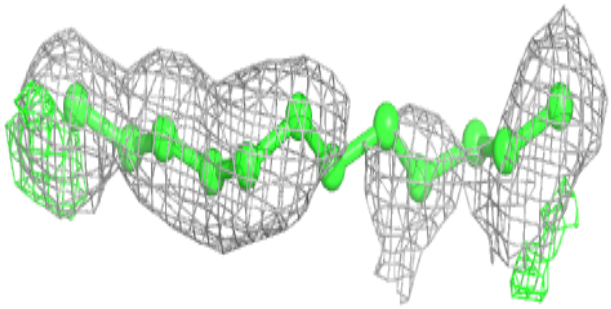


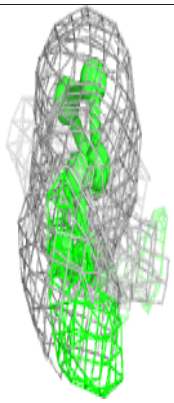


Electron density around OLC A 504:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







Electron density around OLC A 511:

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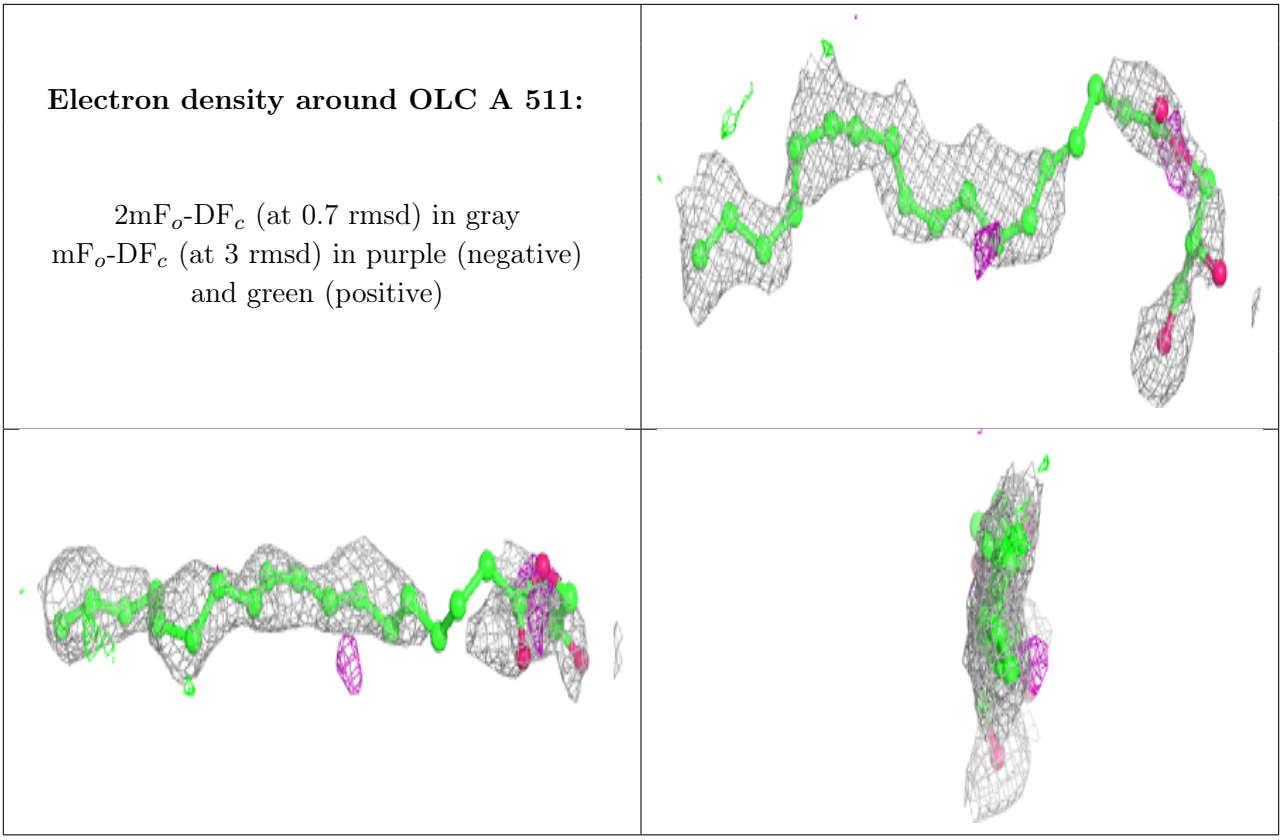
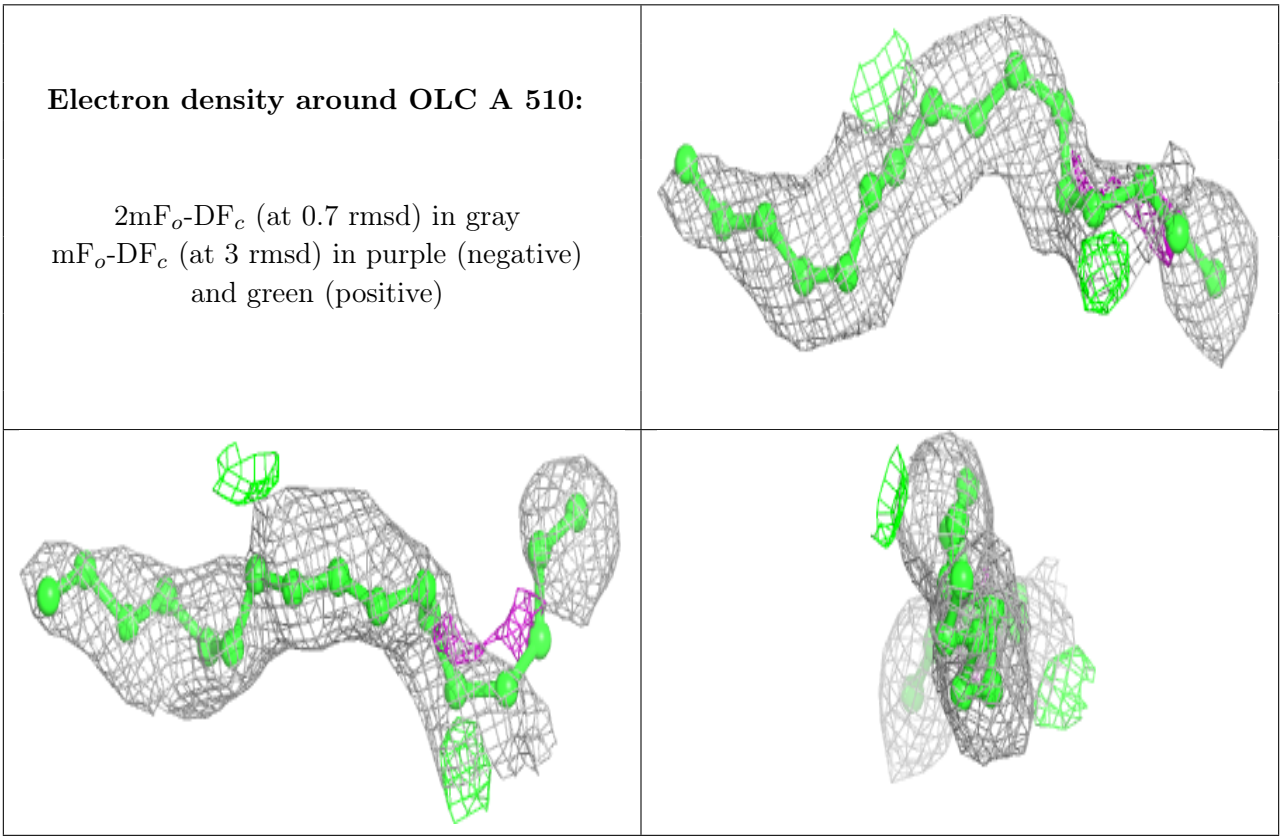
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



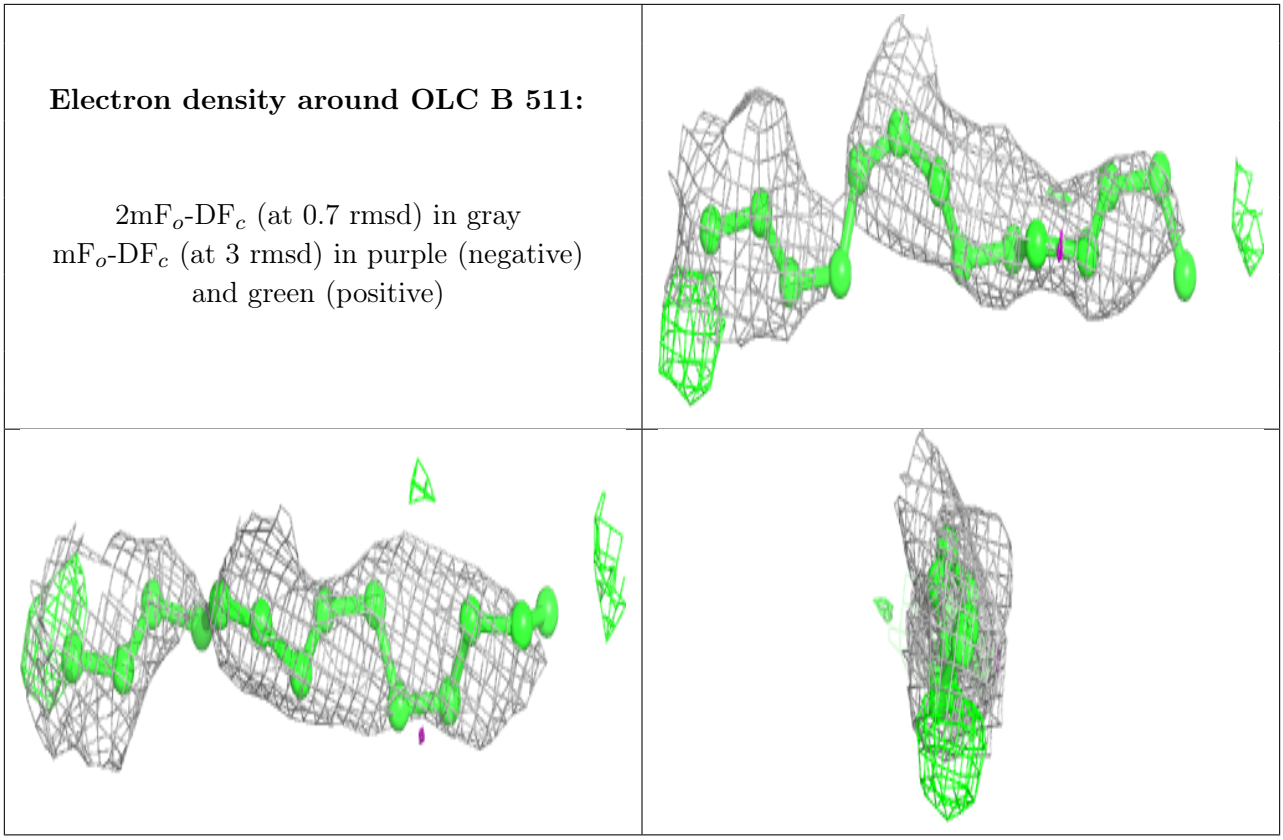
Electron density around OLC A 510:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



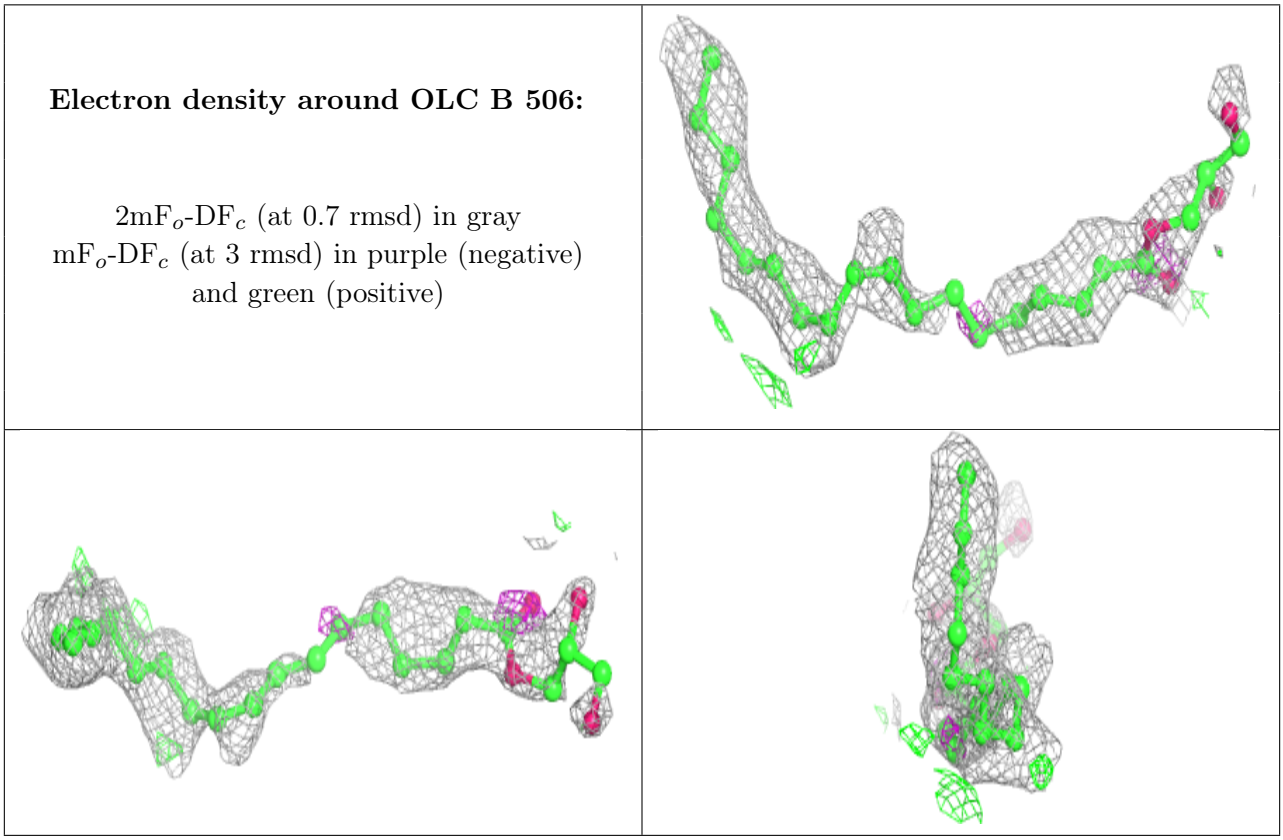
Electron density around OLC B 511:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



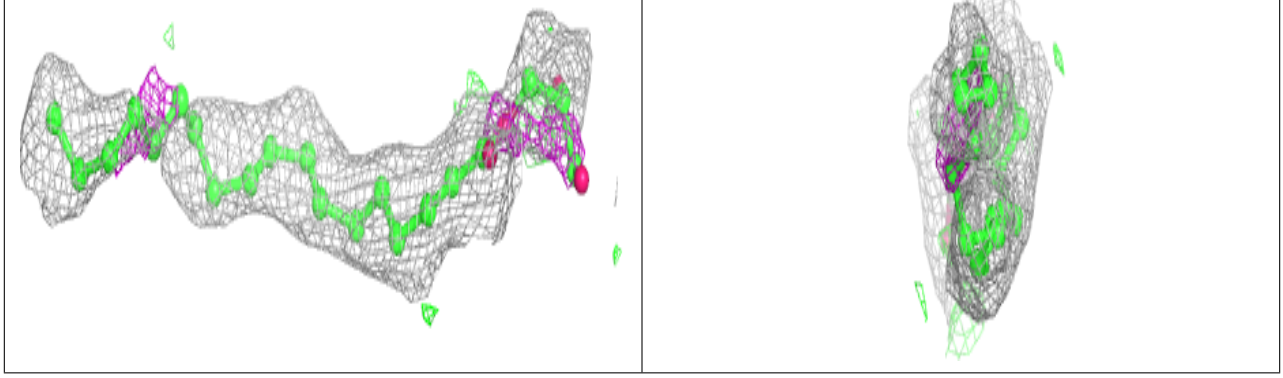
Electron density around OLC B 506:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



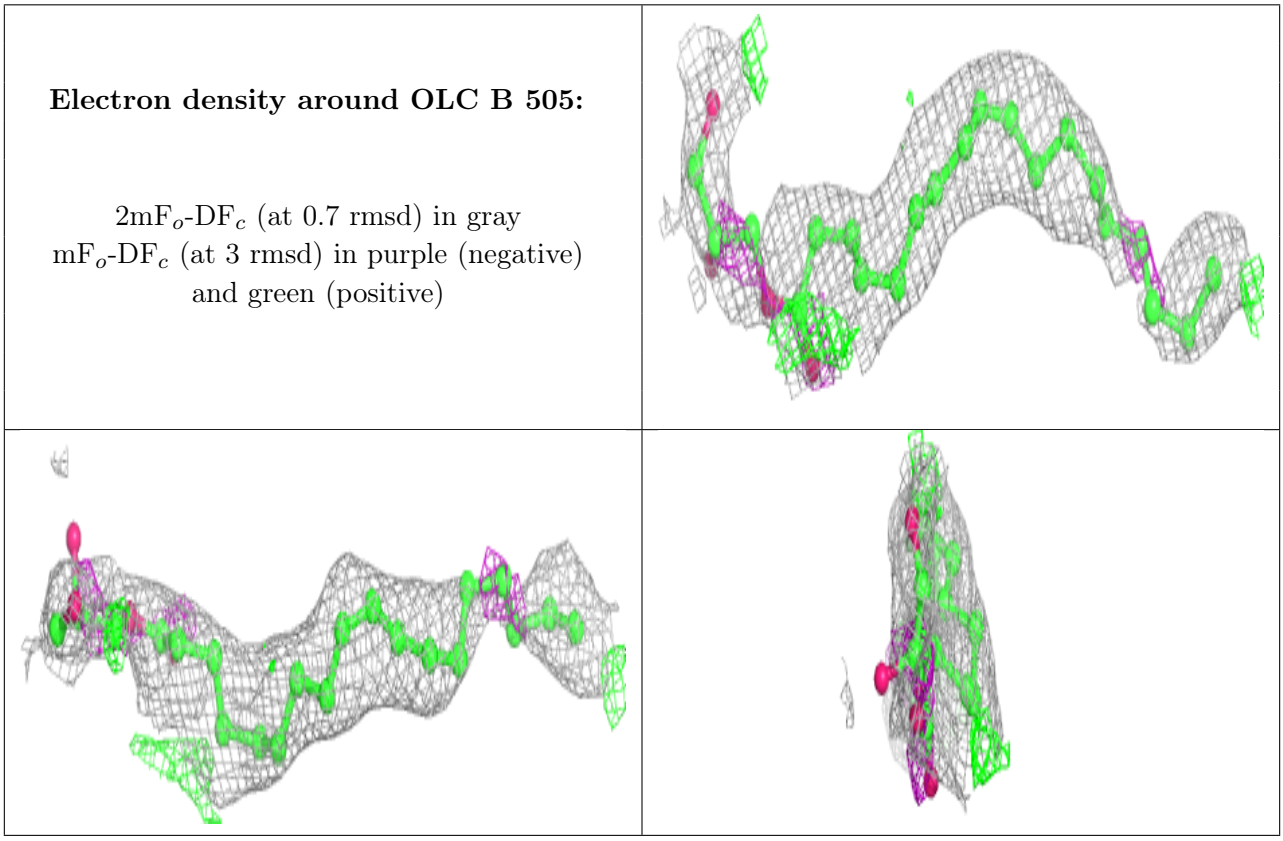
Electron density around OLC A 506:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



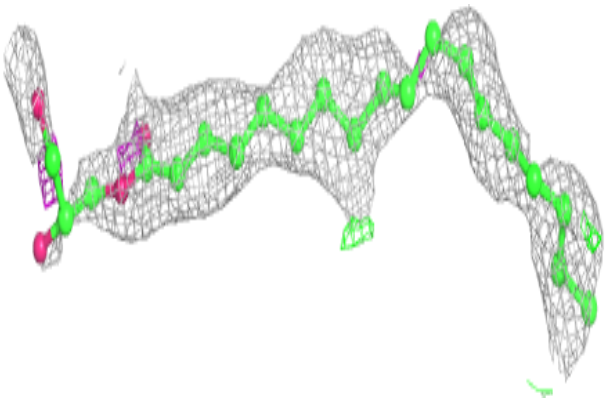
Electron density around OLC B 505:

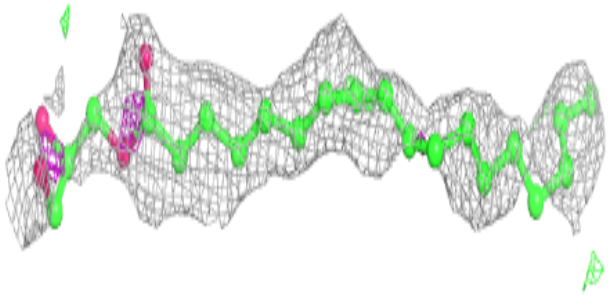
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

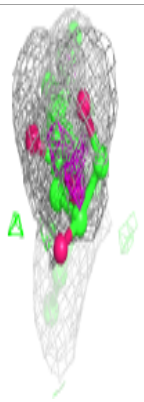


Electron density around OLC B 507:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

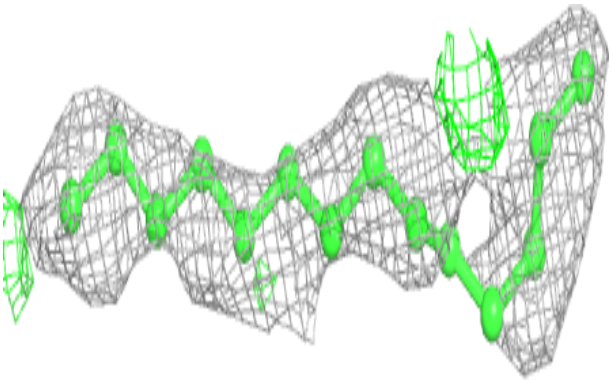


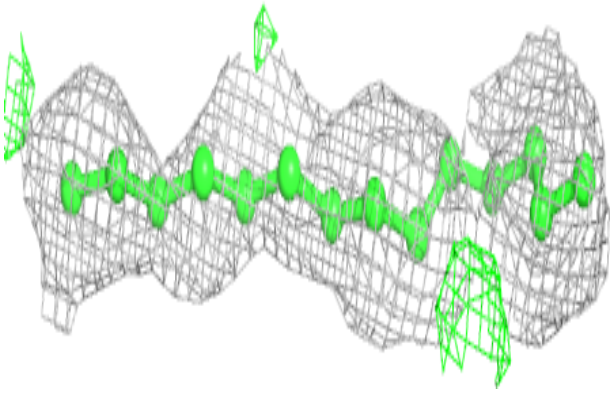


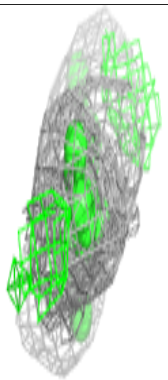


Electron density around OLC B 503:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

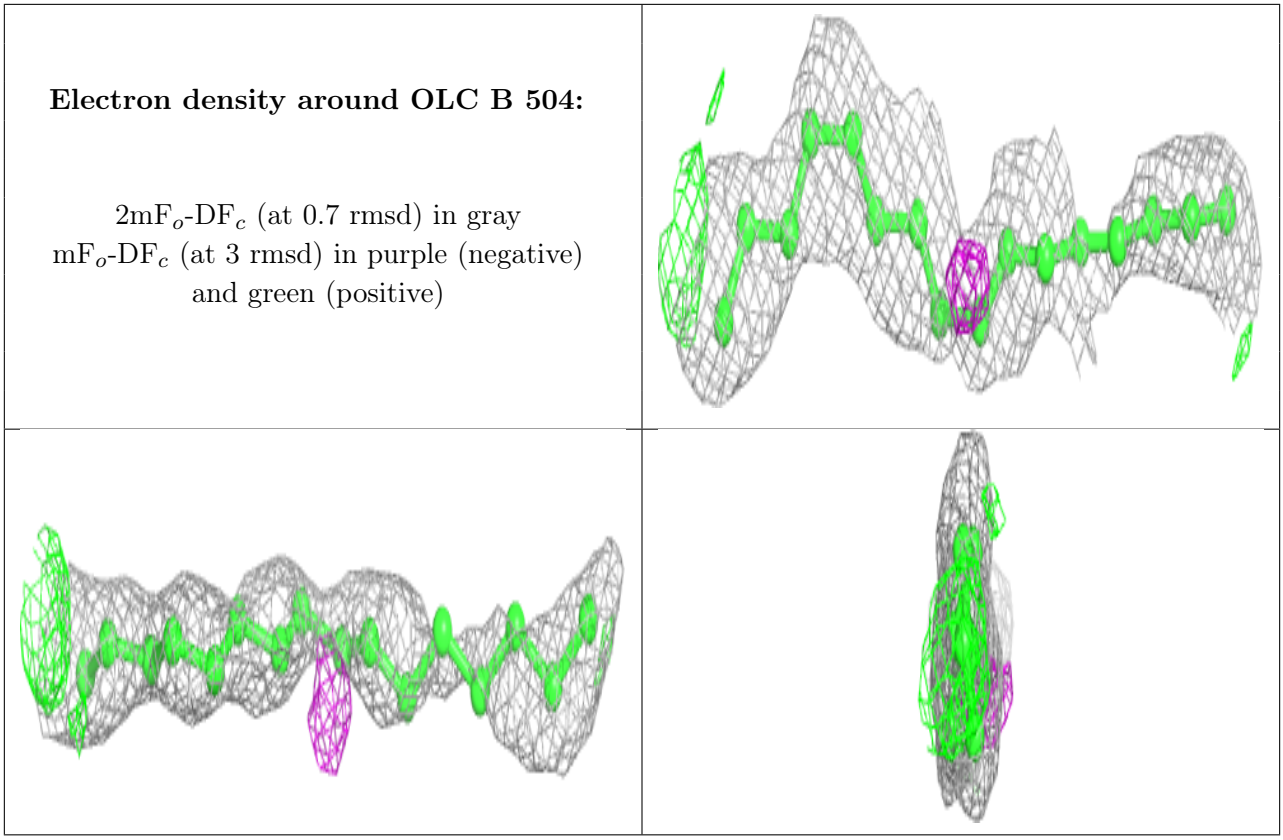






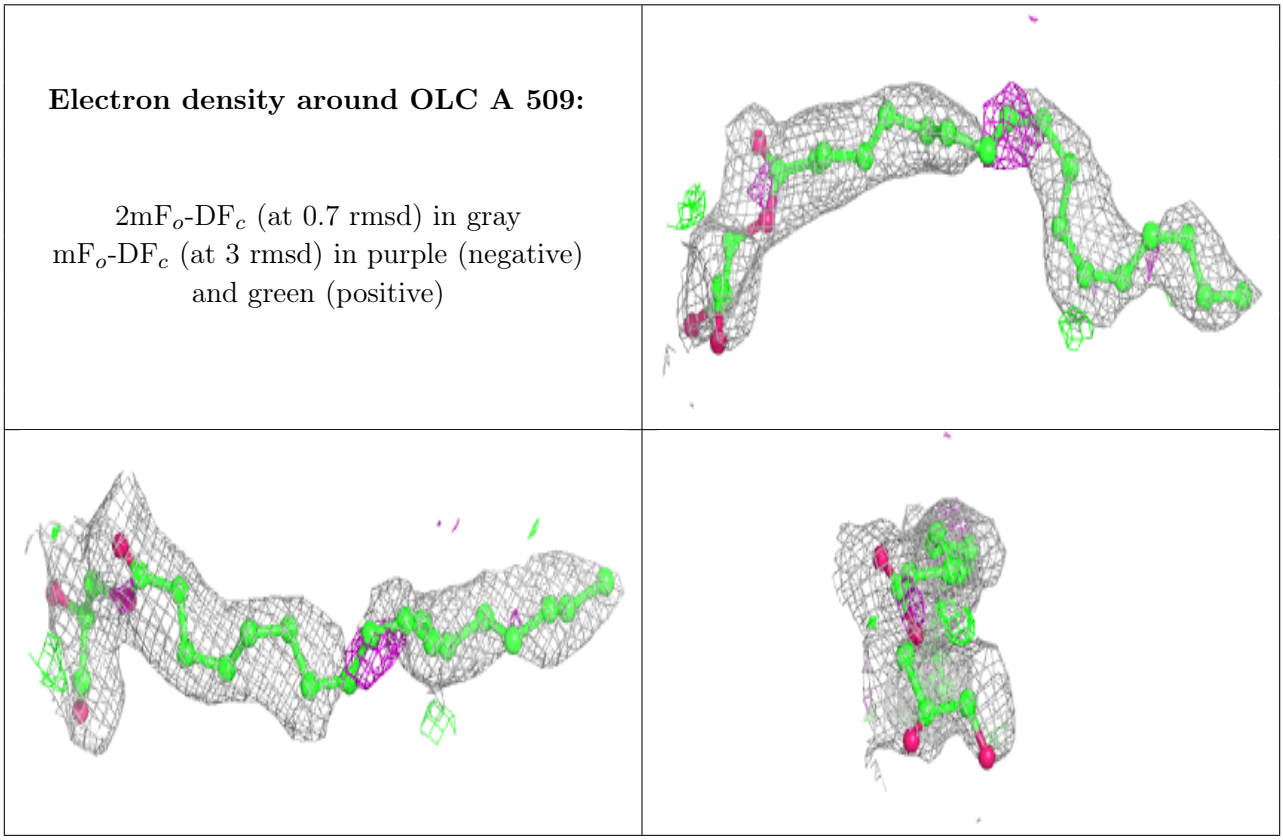
Electron density around OLC B 504:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



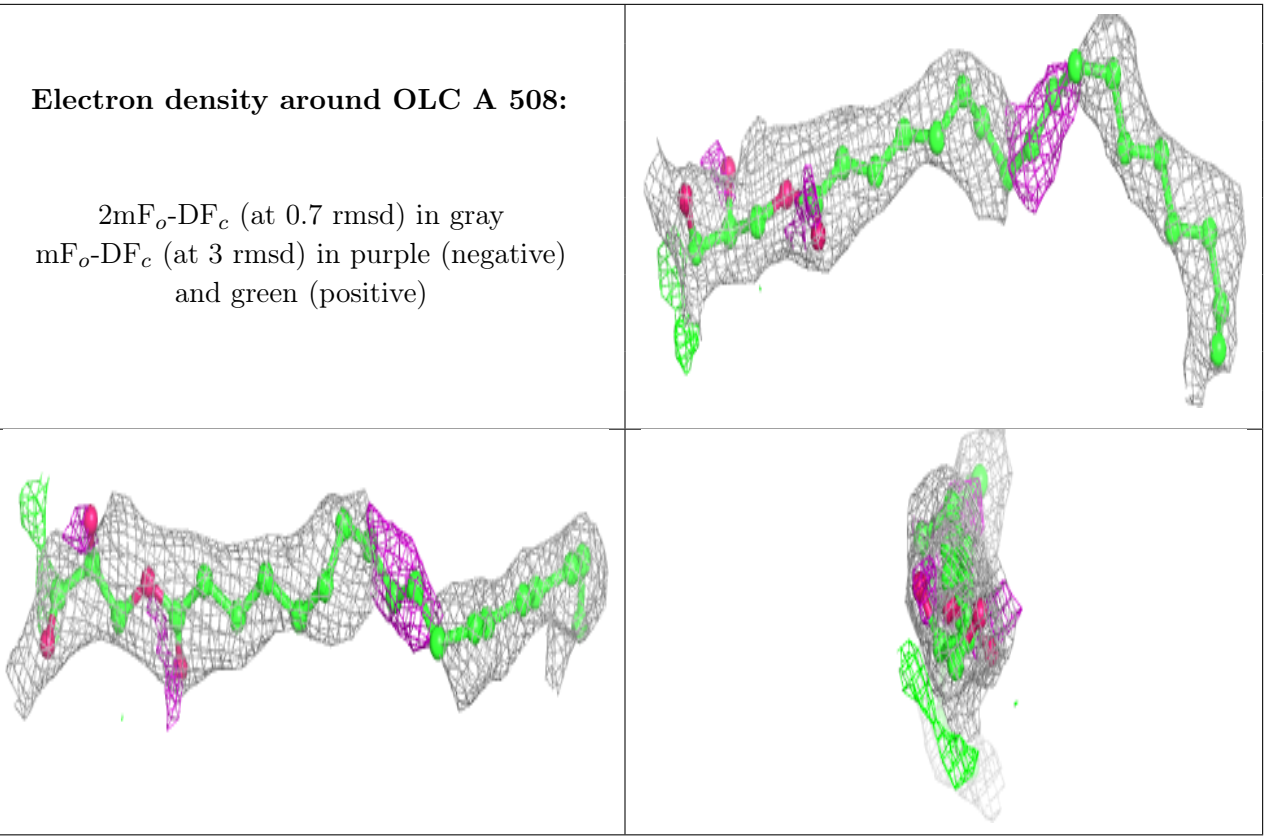
Electron density around OLC A 509:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



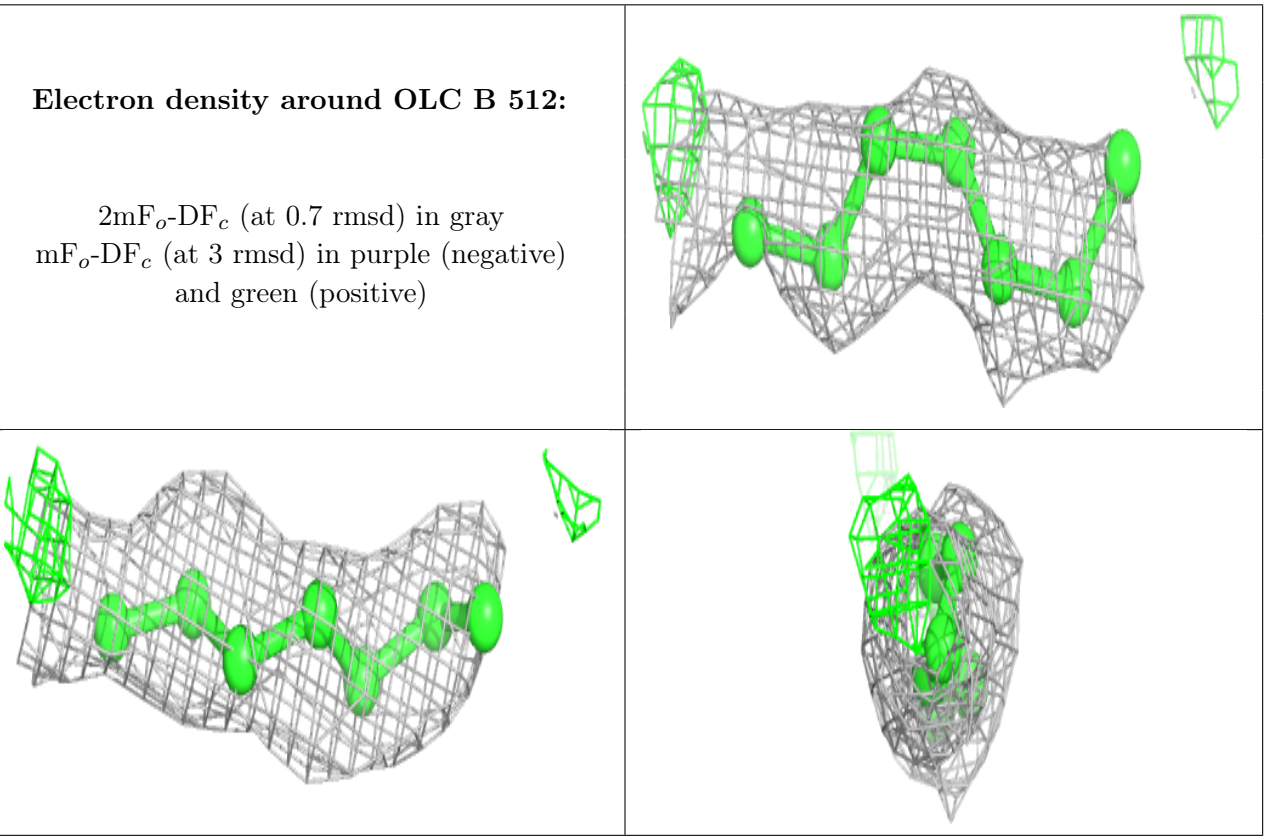
Electron density around OLC A 508:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



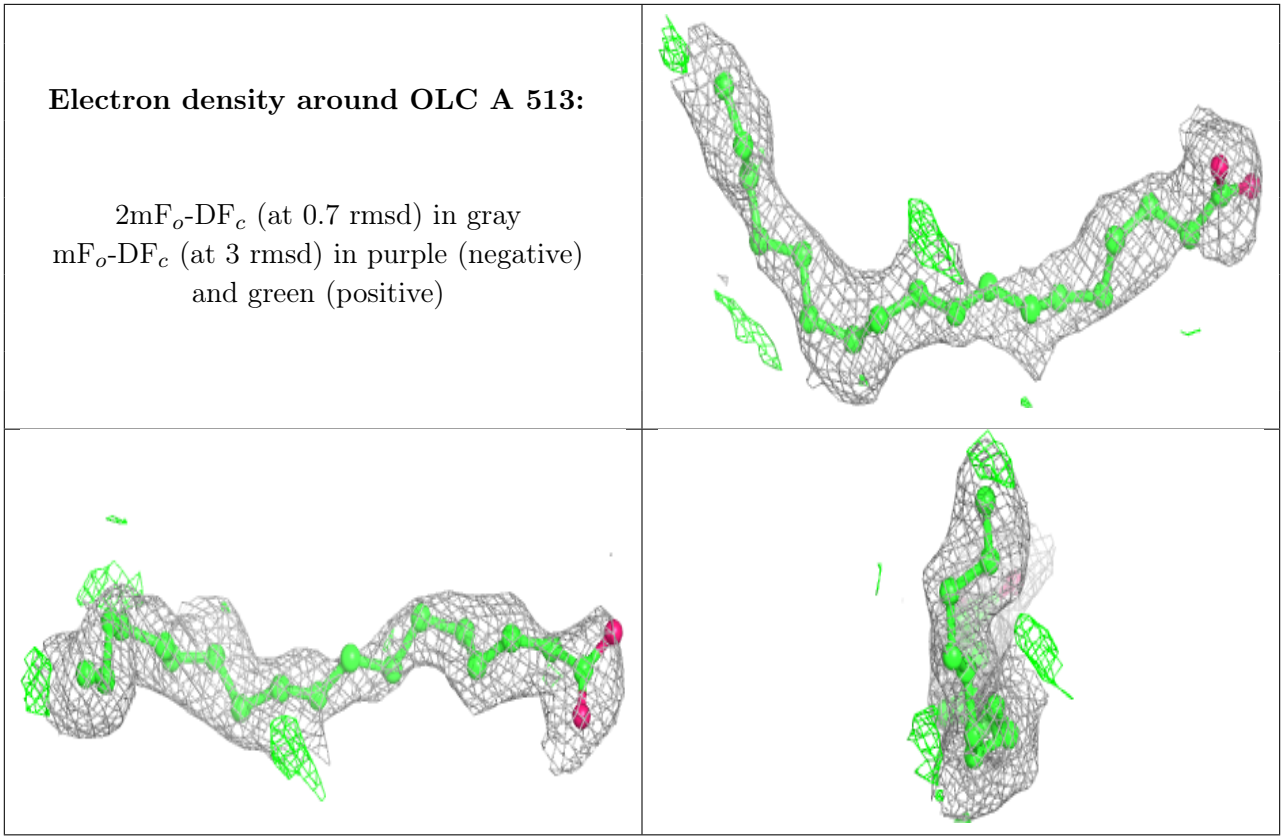
Electron density around OLC B 512:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



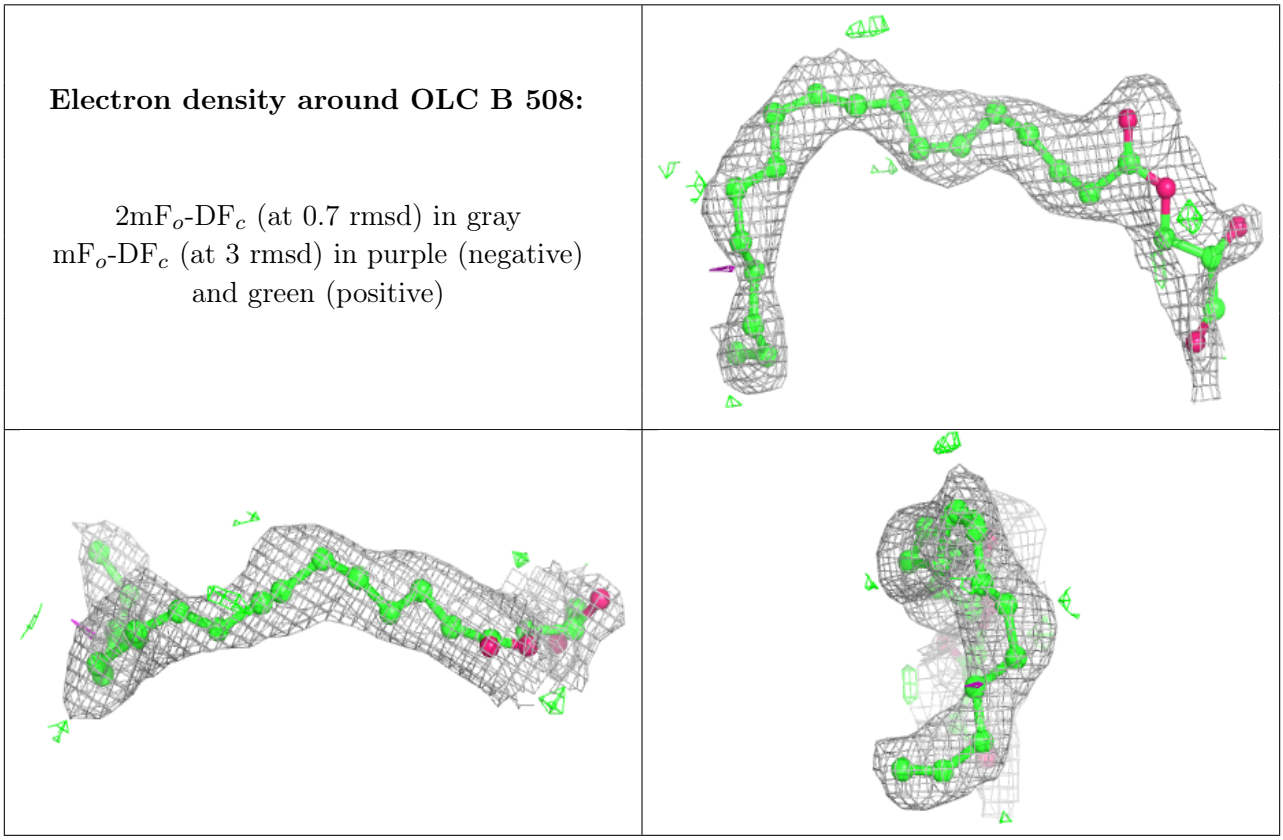
Electron density around OLC A 513:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



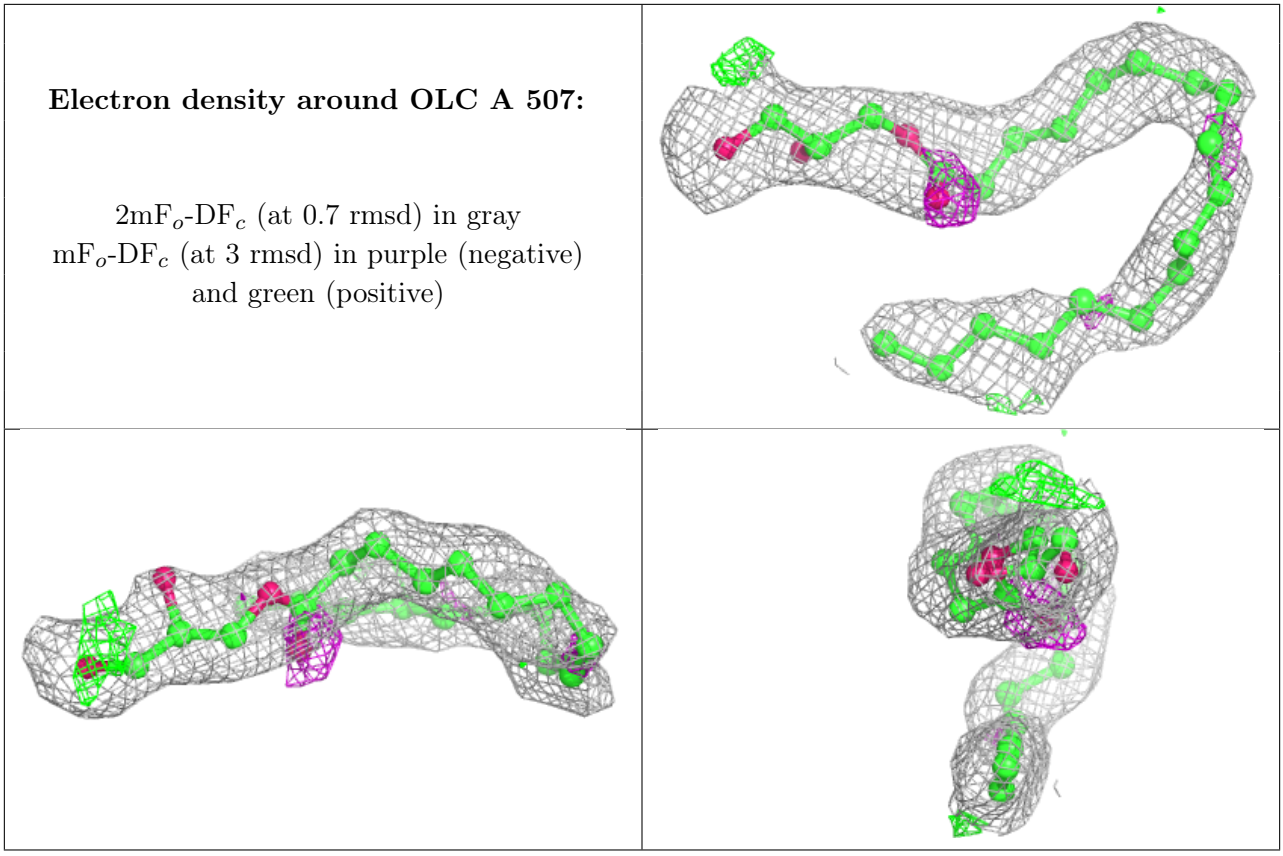
Electron density around OLC B 508:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



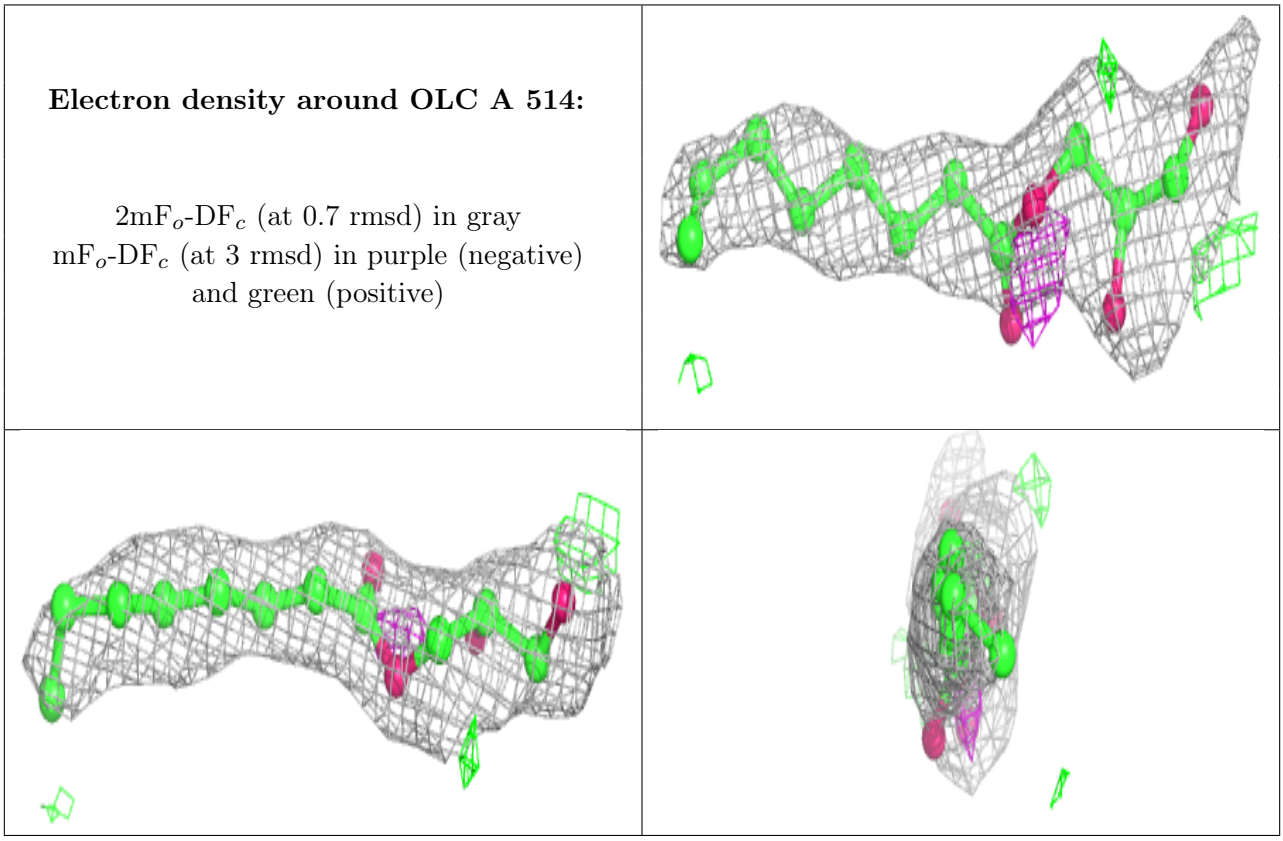
Electron density around OLC A 507:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



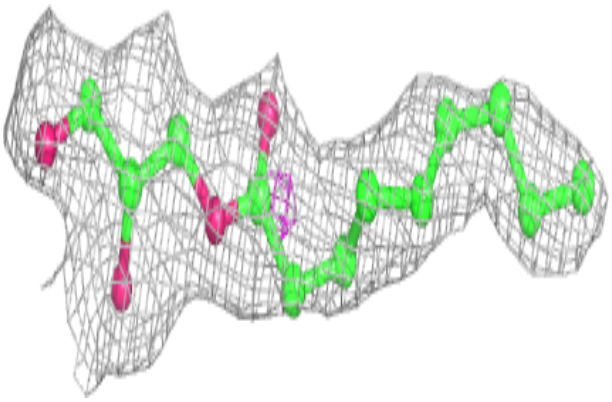
Electron density around OLC A 514:

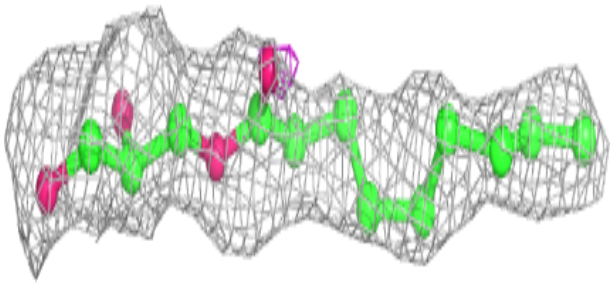
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

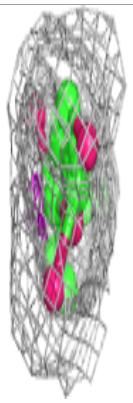


Electron density around OLC B 510:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

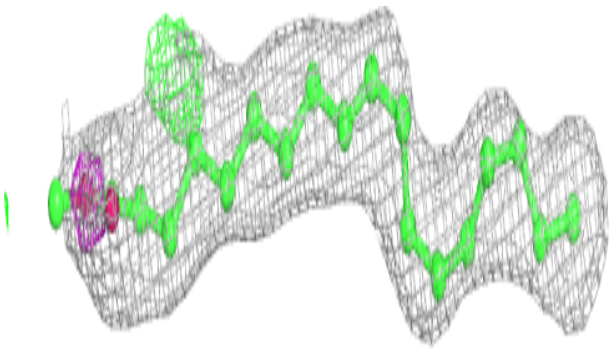


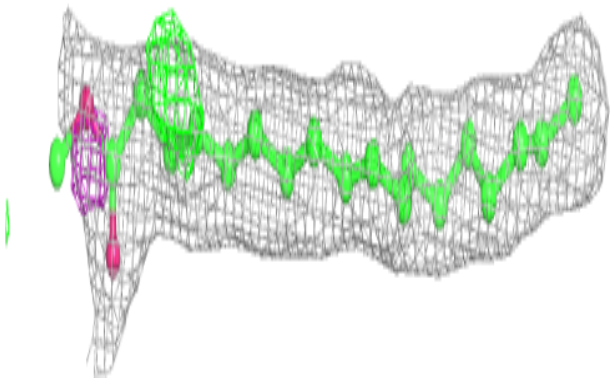


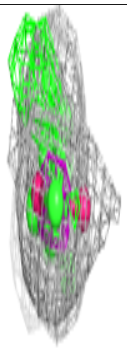


Electron density around OLC B 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

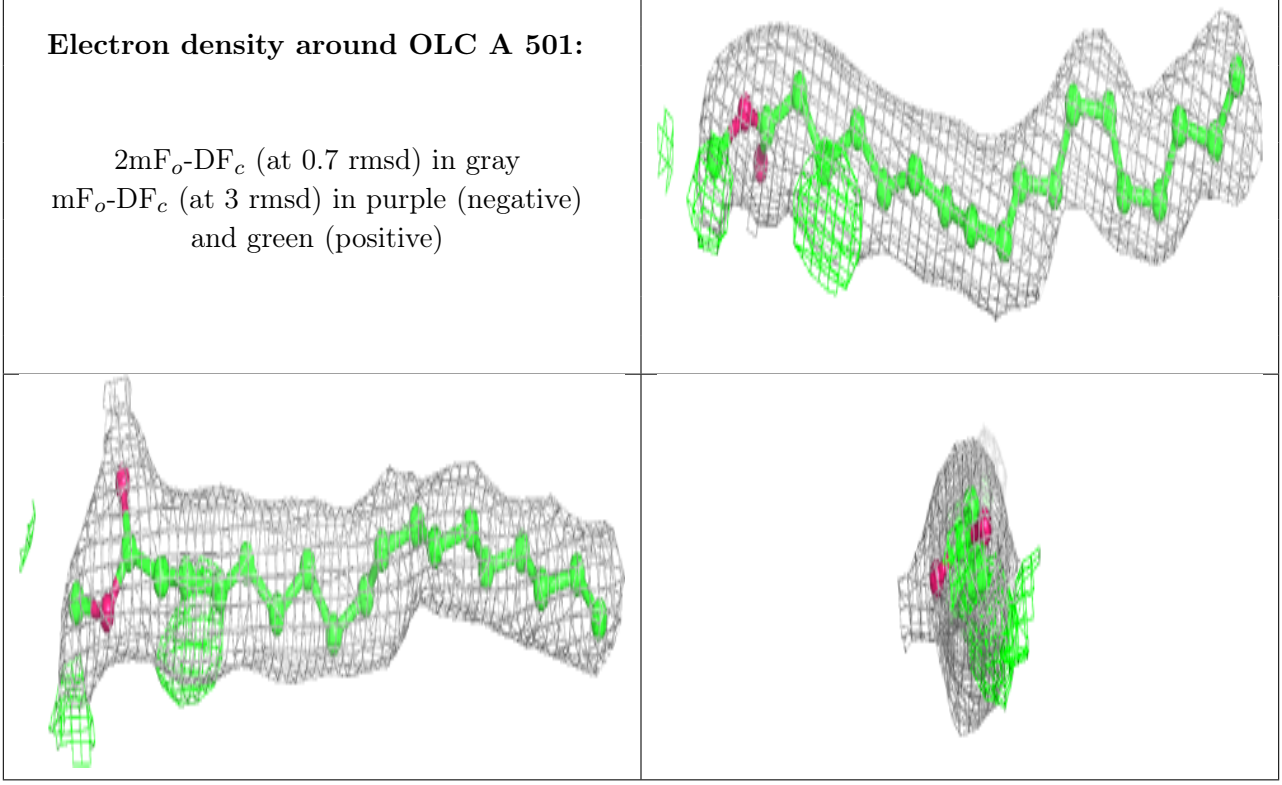






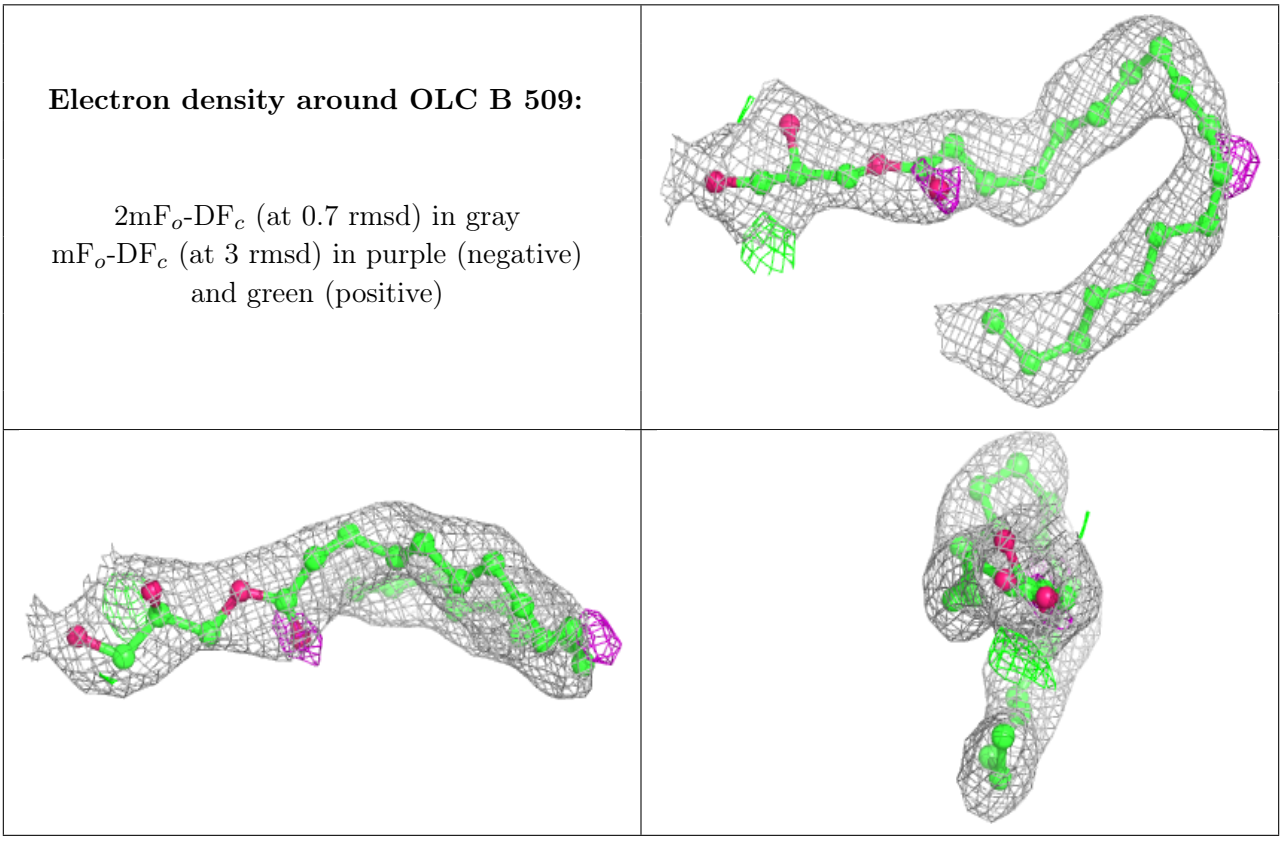
Electron density around OLC A 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



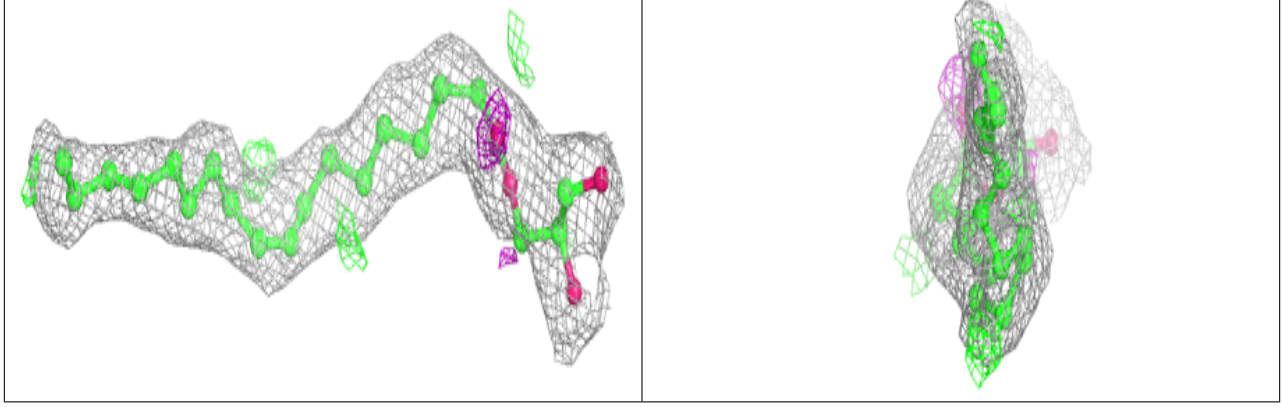
Electron density around OLC B 509:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



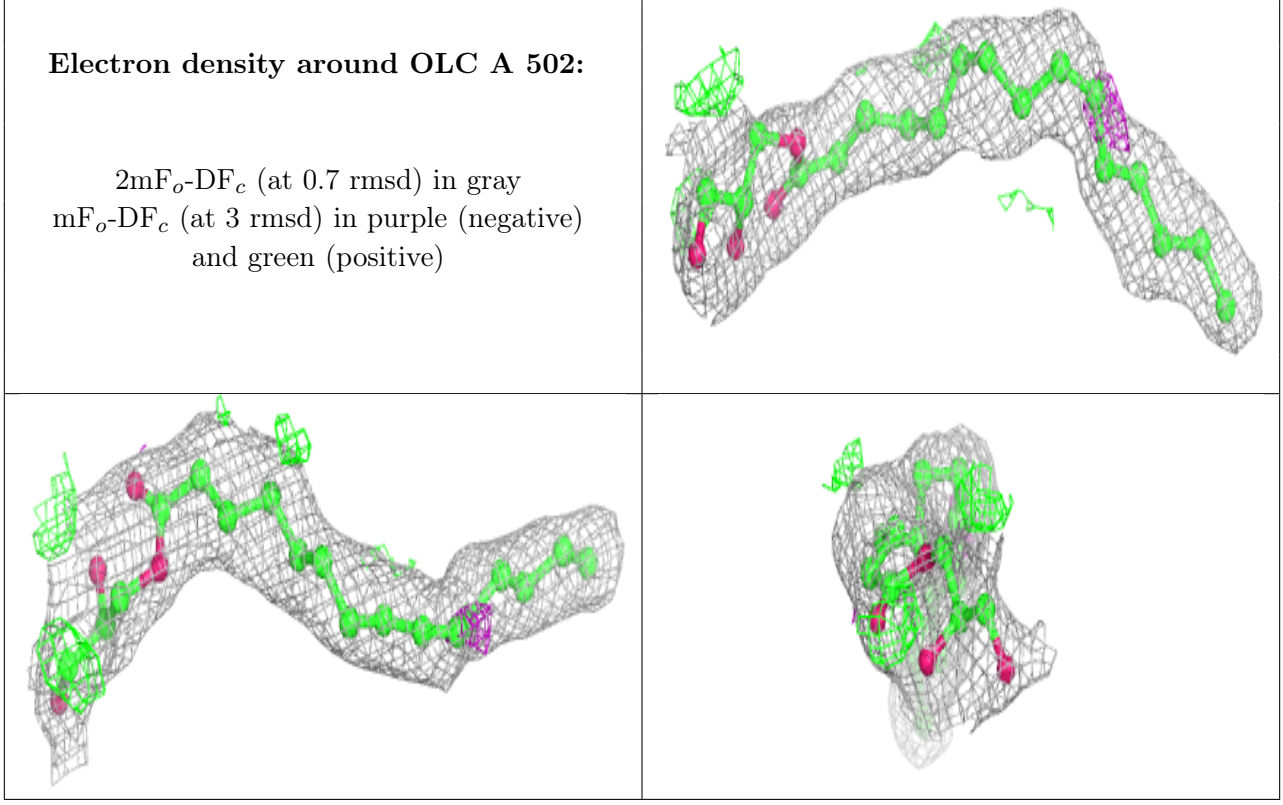
Electron density around OLC B 502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around OLC A 502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.